Appendix A

List of Publications (A–D) and Research Associates (E) of Bernhard Wunderlich

A: Written at The University of Tennessee and Oak Ridge National Laboratory 1988–2010 *

November 25, 2009

A-23: 2010 Publications (4)

600 B. Wunderlich, A Science Career Against All Odds, (A Life of Survival, Study, Teaching and Travel in the 20th Century). 708 Pages and 691 Figures, to be published 2010, Springer, Berlin.

590 B. Wunderlich, Global and Local Phase/Molecular Nucleation, Solid/Mobil, and Order/Disorder Transitions in Macromolecular Systems. (To be based on a projected lecture to be given at the 11th Lähnwitz Seminar in Rostock-Warnemünde, June 6–11, 2010), *Thermochim. Acta*, to be published in 2011.

588 The Role of Mesophases in Polyethylene, Polypropylene and Poly(1-butene) (in cooperation with C. Schick, R. Androsch, and M. L. Di Lorenzo) *To be written, in* (2010).

586b B. Wunderlich, Thermodynamic Description of Condensed Phases. *Journal Thermal Analysis and Calorimetry*, submitted November (2009) for publication in 2010.

A-22: 2009 Publications (7)

589 M. L. Di Lorenzo, M. C. Righetti, and B. Wunderlich, Influence of Crystal Polymorphism on the Three-phase Structure and on the Thermal Properties of Isotactic Poly(1-butene). *Macromolecules* in print (2009).

587 M. L. Di Lorenzo, M. C. Righetti, and B. Wunderlich, Thermal Analysis of the Three-phase Structure of Isotactic Poly(1-butene). *37th NATAS Conf. on Thermal Analysis and Applications, in Lubbock, TX*, Sept. 20–23, E. Schoch, editor. CD edition, **37,** 10 pages (2009).

586a B. Wunderlich, Thermodynamic Description of Condensed Phases. *37th NATAS Conf. on Thermal Analysis and Applications, in Lubbock, TX*, Sept. 20–23, E. Schoch, editor. CD edition, **37,** 15 pages (2009).

585 B. Wunderlich, Quasi-isothermal Temperature-modulated Differential Scanning Calorimetry (TMDSC) for the Separation of Reversible and Irreversible Thermodynamic Changes in Glass Transition and Melting Ranges of Flexible Macromolecules, *Pure and Applied Chemistry*, **81**, 1931–1952 (2009); (doi: 10.1351/PAC-CON-08-07-05) [Proceedings of the ICCT 08, Warszawa, Poland, August 3–8).].

584 B. Wunderlich, Thermodynamics and Properties of Nanophases, *Thermochim. Acta*, **492**, 2–15 (2009); doi: 10.1016/j.tca.2008.10.026. [Based on the Plenary Lecture at the 10th Lähnwitz Seminar, on 'Calorimetry in a Nano-scale' in Rostock-Warnemünde, Germany, June 9–12, 2008.]

582 B. Wunderlich, The Phases Between Solid and Liquid, Characterized by Thermal Analysis. In J. Šesták, M. Holeček, and J. Málek, Some Thermodynamic, Structural and Behavioral Aspects of Materials Accentuating Non-crystalline States; OPS Pilsen, Czech Republic, pp. 118–138 (2009), ISBN 978-80-87269-06-0.

580. B. Wunderlich, Thermal Analysis of the Condensed Phases In P. Hubík, J. Mareš, and J. Šesták, eds. Glassy, Amorphous, and Disordered Materials: Thermal Analysis, Structure and Properties; Springer, Berlin, projected for, 2009.

A-21: 2008 Publications (4)

583 B. Wunderlich, Temperature-modulated Calorimetry of Poly[oxy(benzoate-*co*-naphthoate)]s as Examples of Rotationally Hindered Polymers, *Proc. NATAS Ann. Conf. on Thermal Analysis and Applications* (2008) (Atlantic City, GA, Aug. 18–20) **36,** 2/1–2/11. PNACCS AN 2009:240194

581 B. Wunderlich, Thermodynamics and Kinetics of Crystallization of Flexible Molecules, *J. Polymer Sci., Part B: Polymer Physics*, **46**, 2647–2659 (2008). [See also the extended abstract as publication 577].

578b. B. Wunderlich, Thermal Properties of Aliphatic Nylons and Their Link to Crystal Structure and Molecular Motion, *Journal of Thermal Analysis and Calorimetry*, **93**, 7–17 (2008).

569. J. Ma, A. Habenschuss, and B. Wunderlich, Modulated Calorimetry of Poly(1,4-oxybenzoate) and Poly(2,6-oxynaphthoate) and their Copolymers, *Thermochim. Acta*, **471**, 90–96 (2008).

A-20: 2007 Publications (12)

579. B. Wunderlich, The Differences in Structural and Thermal Properties Between Random and Precisely Structured Copolymers of Polyolefins. (PPT presentation). *Proceedings of the Meeting on Advances in Polyolefins:*, in Santa Rosa, CA, September 23–26 (2007).

578a. B. Wunderlich, Thermal Properties of Aliphatic Nylons and Their Link to Crystal Structure and Molecular Motion. *Proc. NATAS Conf. on Thermal Analysis and Applications* (2007) (East Lansing, MI, Aug. 26–29), **35** #785/1–10. PNACS: 1156903.

577 B. Wunderlich, Fifty-year Development of the Understanding of Motion and Defects in Macromolecular Crystals Based on Thermal Analysis, Structure Analysis, and Computer Simulation. 234th ACS Natl. Meeting, Boston, August 19–23, 2007. *PMSE Preprints*, **97**, 70–73, (2007). See also publication 581.

576. B. Wunderlich, The Use of Modern DSC for the Study of Metastastable and Unstable Materials, *American Pharmaceutical Review*, **10**/3, 99–103 (2007).

575b. B. Wunderlich, Thermal Analysis of Macromolecules, A Personal Review, *Journal of Thermal Analysis and Calorimetry*, **89**, 321–356 (2007), ISSN 1572-8943 (Online). [An update and extension of publication 407, see also Appendix B of publication 600 for an extension to 2010.]

574b. B. Wunderlich, Calorimetry of Nanophases of Macromolecules, *Int. J. of Thermophys.*, **28**, 958–967 (2007).

573. W. Qiu, A. Habenschuss, and B. Wunderlich, The Phase Structures of Nylon 6.6 as Studied by Temperature-modulated Calorimetry and Their Link to X-ray Structure and Molecular Motion. *Polymer*, **48**, 1641–1650 (2007).

570. B. Wunderlich, The Glass Transition as Key to Identify Solid Phases. *J. Appl. Polymer Sci.*, **105**, 49–59 (2007).

567. R. Androsch and B. Wunderlich, Scanning Calorimetry, in K. Matyjaszewski, Y. Gnanou, and L. Laibler, eds. "Macromolecular Engineering," Vol. 3, Chapter 14. WIILEY-VCH, Weinheim, pp. 1827–1880, 2007.

565. W. Qiu, M. Pyda, E. Nowak-Pyda, A. Habenschuss, and B. Wunderlich, Reversible Melting and Crystallization of High Molar Mass Poly(oxyethylene) Measured by Temperature-modulated DSC and X-ray Diffraction, *J. Polymer Sci., Part B: Polymer Physics,* **45**, 475–489 (2007).

528 B. Wunderlich, 100 Years Research on Supercooling and Superheating, *Thermochim. Acta*, **461**, 4–13 (2007). [Proceedings of the 9th Lähnwitz Seminar on 'Transitions Far From Equilibrium—Superheating and Supercooling.' Rostock-Warnemünde, Germany, May 28–June 1, 2006.]

276d. B. Wunderlich and M. Pyda, Thermodynamic Properties of Polymers in J. I. Kroschwitz, ed. "Encyclopedia of Polymer Science and Engineering," Concise Third Edition, 43 pp., John Wiley & Sons, New York, DOI: 10.1002/0471440264. PST 369 (2007). [Also at: www.mrw.interscience.wiley.com/epst.]

A-20: 2006 Publications (12)

575a. B. Wunderlich, Thermal Analysis of Macromolecules, A Personal Review. (Update and extension of publication 407.) *Proc. 34th NATAS Conf. on Thermal Analysis and Applications, in Bowling Green, KY*, Aug. 6–9, I. Vitaz, M. J. Rich, and K. E. Schoch, edts. CD edition, **34,** 003.11.567/1–003.11.567/47 (2006). CODEN: PNACCS AN 2006:1131721 CAPLUS. [For details, see publication 575b and a further update to 2010 is given as Appendix B in publication 600.]

574a. B. Wunderlich, The Calorimetry of Nanophases of Macromolecules, *Proceedings of the THERMO International 2006 in Boulder, CO,* 7/30–8/4, 2006; Gary Hardin, Chris Muzny, and Dan Friend, editors, p850.pdf. [9-page proceedings paper, for more details see publication 574b.]

572. W. Qiu and B. Wunderlich, Reversible Melting of High Molar Mass Poly(oxyethylene). *Thermochim. Acta*, **448,** 136–146 (2006); doi:10.1016/j.tca.2006.07.005.

571. W. Qiu, M. Pyda, A. Habenschuss, K. B. Wagener, and B. Wunderlich, Crystallization and Melting of a Branched Polyethylene with Precisely Controlled Chemical Structure. *J. Polymer Sci., Part B: Polymer Physics,* **44**, 3461–3474 (2006).

568b. R. Androsch and B. Wunderlich, Effect of Crystallinity and Crystal Perfection on the Rigid-amorphous Structure in Cold-crystallized Poly(ethylene yerephthalate), *Proc. 34th NATAS Conf. in Bowling Green, KY,* Aug. 6–9, I. Vitaz, M. J. Rich, and K. E. Schoch, edts. CD edition, **34,** 005-11-587/1 (2006). [One-page Abstract.]

566. W. Qiu, J. Sworen, M. Pyda, E. Nowak-Pyda, A. Habenschuss, K. B. Wagener, B. Wunderlich, Effect of the Precise Branching of Polyethylene at each 21st CH_2 Group on its Phase Transitions, Crystal Structure, and Morphology, *Macromolecules*, **39**, 204–217. (2006).

563b B. Wunderlich, The Glass Transition of Polymer Crystals. *Thermochim. Acta*, **446**, 128–134 (2006).

562b. B. Wunderlich, The Contributions of MDSC to the Understanding of the Thermodynamics of Polymers. *Journal of Thermal Analysis and Calorim.* **85**, 179–187 (2006).

558. A. Habenschuss, M. Varma-Nair, Y.-K. Kwon, J. Ma, and B. Wunderlich, The Phase Diagram of Poly(4-hydroxybenzoic Acid) and Poly(2,6-hydroxynaphthoic Acid) and their Copolymers from X-ray Diffraction and Thermal Analysis, *Polymer*, **47**, 2369–2380 (2006).

549b. M. Pyda, E. Nowak-Pyda, and B. Wunderlich, The Heat Capacity of Polyethylene Fibers Measured by Multi-frequency Temperature-modulated Calorimetry, *Thermochim. Acta*, **442**, 35–41 (2006).

548b,c M. Pyda, E. Nowak-Pyda, J. Heeg, H. Huth, A. A. Minakov, M. L. Di Lorenzo, C. Schick, and B. Wunderlich, Melting and Crystallization of Poly(butylene terephthalate) by Temperature-modulated and Superfast Calorimetry, *J. Polymer Sci., Part B: Polymer Physics.*, **44**, 1364–1377 (2006). [(c) One-page abstract: *Proc. 34th NATAS Conf. in Bowling Green, KY*, Aug. 6–9, I. Vitaz, M. J. Rich, and K. E. Schoch, edts. CD edition, **34,** 004-11-791/1 (2006).

454a. B. Wunderlich, The Application of MTDSC to Polymer Melting, in M. Reading, and D. J. Hourston, eds., "Modulated Temperature Differential Scanning Calorimetry." Springer, Dordrecht, The Netherlands, 2006, pp. 217–319.

A-18: 2005 Publications (20)

568a. R. Androsch and B. Wunderlich, The Link Between Rigid-amorphous Fraction and Crystal Perfection in Cold-crystallized Poly(ethylene terephthalate), *Polymer* **46**, 12556–12566 (2005).

564a,b M. Pyda, K. Van Durme, B. Wunderlich and B. Van Mele, Heat Capacity of Poly(vinyl methyl ether) in the Presence and Absence of Water, *Proc. 33rd NATAS Conf. in Universal City, CA*, Sept. 18–21, M. J. Rich, edt. CD edition, **33,** 138.47.550/1–10 (2005). [(9b) Feature Article in *NATAS Notes*, **37(4)**, 7–13 (2005), based on publ 564 a.]

563a B. Wunderlich, The Glass Transition of Polymer Crystals. *Proc. 33rd NATAS Conf. in Universal City, CA*, Sept. 18–21, M. J. Rich, edt. CD edition, **33,** 127.47.165/1–9 (2005).

562a. B. Wunderlich, The Contributions of MDSC to the Understanding of the Thermodynamics of Polymers. *Proc. 33rd NATAS Conf. in Universal City, CA*, Sept. 18–21, M. J. Rich, edt. CD edition, **33,** 025-39,477/1–10 (2005).

561. R. Androsch, B. Wunderlich, and H.-J. Radusch, Analysis of Reversible Melting in Polytetrafluoroethylene, *Journal of Thermal Analysis and Calorimetry*, **79**, 615–622 (2005).

560. B. Wunderlich, Thermal Analysis of Materials. A computer-assisted lecture course of 36 lectures. Updated and changed to newly developed presentation software, published via the Internet (2005–2007). Available by downloading through the internet sites: http://www.scite.eu (under 'Books and more'), http://athas.prz.rzeszow.pl (under 'Teaching'), and http://www.evitherm.org/index.asp (from their home page, go to 'Thermal analysis & calorimetry').

559. W. Qiu, M. Pyda, E. Nowak-Pyda, A. Habenschuss, and B. Wunderlich, Reversibility Between Glass and Melting Transitions of Poly(oxyethylene), *Macromolecules*, **38**, 8454–8467 (2005).

557. M. Pyda, K. Van Durme, B. Wunderlich, and B. Van Mele, Heat Capacity of Poly(vinyl methyl ether), *J. Polymer Sci., Part B: Polymer Physics*, **43**, 2141–2153 (2005).

556a,b B. Wunderlich, Effect of Decoupling of Molecular Segments, Microscopic Stress-transfer, and Confinement of the Nanophases in Semicrystalline Polymers. Feature Article in: *Macromol. Rapid Comm.*, **26**, 1521–1531 (2005). Preprinted as 556a: Keynote lecture in Symposium 8 "Morphology and Structure Development." *Conf. Proc. PPS21 Meeting in Leipzig, Germany*, June 19–23 (2005). Martin-Luther-University, Leipzig, Germany, H.-J. Radusch, editor.

555. B. Wunderlich, Discussion of Problems of Nonequilibrium Thermodynamics of Polymers as Presented in the Paper by Sommer and Reiter. *Thermochim. Acta*, **432**, 148–152 (2005).

554a,b Pyda, M., Relaxation Processes of the Amorphous and Semicrystalline Biodegradable Poly(lactic acid) by Temperature-modulated Calorimetry. *ACS Spring Meeting in San Diego, CA*, March 13 to 17. *Proc. of Polymeric Materials Science and Engineering.* **92**, 570–571 (2005); 554b: Marek Pyda, E. Nowak-Pyda, and B. Wunderlich, Characterization of the Amorphous and Semicrystalline Biodegradable Poly(lactic acid) by Temperature-modulated Calorimetry. Printed version of the Lecture in Symposium 10 given by M. Pyda (SL-10.2, 11 pp): "Natural Based und Biodegradable Polymers." *Conference Proceedings of the PPS21 Meeting in Leipzig, Germany*, June 19–23 (2005). Martin-Luther-University, Leipzig, Germany, H.-J. Radusch, editor, ISBN 3-86010-784-4.

553. B. Wunderlich, Effect of Confinement of the Amorphous Phase of Polymers in Semicrystalline Polymers. *ACS Spring Meeting in San Diego, CA*, March 13 to 17. *Proc. of Polymeric Materials: Science and Engineering.* **92**. 574–575 (2005).

551. B. Wunderlich, The Influence of the Surface on the Thermodynamics of the Melting and Glass Transition of Films and Fibers. *Thermochim. Acta*, **432**, 127–134 (2005). [Based on a lecture given at the 8th Lähnwitz Seminar on 'Thermodynamics and Calorimetry of Thin Films' in Warnemünde, Germany, June 6–10, 2004.]

542b. J. Pak, W. Qiu, M. Pyda, E. Nowak-Pyda, and B. Wunderlich, Can One Measure Precise Heat Capacities with DSC or TMDSC? A Study of the Baseline and Heat-flow-rate Correction, *Journal of Thermal Analysis and Calorimetry*, **82**, 565–574 (2005).

537b,c. M. Pyda and B. Wunderlich, Reversing and Nonreversing Heat Capacity of Poly(lactic acid) in the Glass Transition Region by TMDSC (Temperature-modulated Differential Scanning Calorimetry), *Macromolecules*, **38**,10472–10479 (2005); (c) M. Pyda, E. Nowak-Pyda, and B. Wunderlich, Physical Aging of Amorphous Poly(lactic Acid) by Temperature-modulated Calorimetry. 33rd NATAS Conf., Universal City, CA, Sept. 18–21, M. J. Rich, edt. CD edition, **33,** 135.47.663/1–10 (2005).

521b. R. Androsch, B. Wunderlich, T. Lüpke , and A. Wutzler, Influence of Deformation on Irreversible and Reversible Crystallization of Poly(ethylene-*co*-1-octene). [Abstract only of the Lecture in Symposium No. 8 (SL-8.14, 1 p.): "Morphology and Structure Development." *Conference Proceedings of the PPS21 Meeting in Leipzig, Germany*, June 19–23 (2005) Martin-Luther-University, Leipzig, Germany, H.-J. Radusch, editor.]

500. B. Wunderlich, Thermal Analysis of Polymeric Materials, 894 + xvi pages, 947 figures. Springer, Berlin, 2005. ISBN 978-3-540-23629-0. Online version: www.springer.com/3-540-23629-5.

095&102&123b B. Wunderlich, Macromolecular Physics. Vol. 1,, 568 pp, Crystal Structure, Morphology, Defects. [Look also for the Addendum to Chapter IV (The Defect Crystal), based on publication 359.] Vol. 2, Nucleation, Crystallization, Annealing. Vol. 3, 363 pp, Crystal Melting. Academic Press, New York, 1973, 1976, and 1980. PDF reprints with a new Preface and electronically searchable indices, published in 2005. It is available via the 'Science & Technology' website: www.scite.eu (heading 'Books and more'), and through ATHAS: (http://athas.prz.rzeszow.pl (heading 'Teaching').

A-17: 2004 Publications (16)

552. T. Malmgren, J. Mays, and M. Pyda, Characterization of Biodegradable Poly(lactic acid) by Size Exclusion Chromatography, Differential Refractometry, Light Scattering, and Thermal Analysis, *Proc. 32nd NATAS Conf. in Williamsburg, VA*, Oct. 4–6, M. J. Rich, edt. CD edition, **32,** 070.03.418/1–9 (2004).

550. M. Pyda, Quantitative Thermal Analysis of Carbohydrate-water Systems. In D. Lorinczy, ed. The Nature of Biological Systems as Revealed by Thermal Methods. Kluver, Amsterdam, pp 307–333, 2004.

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548a. M. Pyda, E. Nowak-Pyda, and B. Wunderlich, Thermal Analysis of Quenched Poly(butylene terephthalate) by Temperature-modulated Calorimetry, *Proc. 32nd NATAS Conf. in Williamsburg, VA*, Oct. 4–6, M. J. Rich, edt. CD edition, **32,** 061.16.20.456/1 (2004). [TMDSC only, for full paper see 548b.]

547a,b (b) M. Pyda, X. Buzin, B. Wunderlich, and R. C. Bopp, Thermal Analysis and Morphology of Thin Films of Poly(lactic acid) by Calorimetry and AFM, *Natas Notes*, **35**(4), 17–20 (2004). (a) M. Pyda, E. Nowak-Pyda, and B. Wunderlich, Thermal Analysis and Morphology of Thin Films of Poly(lactic acid) by Calorimetry and AFM, *Proc. 32nd NATAS Conf. in Williamsburg, VA*, Oct. 4–6, M. J. Rich, edt. CD edition, **32,** 165.05.401/1–10 (2004).

546. M. Pyda, Crystallinity of Polymers by Calorimetry and Their Application for Quantitative Thermal Analysis, *Proc. 32nd NATAS Conf. in Williamsburg, VA*, Oct. 4–6, M. J. Rich, edt. CD edition, **32,** 034.02.901/1–10 (2004).

545. B. Wunderlich, The ATHAS Teaching Effort on Thermal Analysis of Polymeric Materials, *Proc. 32nd NATAS Conf. in Williamsburg, VA*, Oct. 4–6, M. J. Rich, edt. CD edition, **32,** 062.03.431/1–10 (2004).

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543. B. Wunderlich, Fast and Super-fast DTA and Calorimetry, *Proc. 32nd NATAS Conf. in Williamsburg, VA*, Oct. 4–6, M. J. Rich, edt. CD edition, **32,** 018.04.569/1–10 (2004)

542a. J. Pak, W Qiu, M. Pyda, E. Nowak-Pyda, and B. Wunderlich, Effect of Pan Deformation on Heat-flow Rate, *Proc. 32nd NATAS Conf. in Williamsburg, VA*, Oct. 4–6, M. J. Rich, edt. CD edition, **32,** 061.12.20.351/1–10 (2004).

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276c. B. Wunderlich and M. Pyda, Thermodynamic Properties of Polymers in J. I. Kroschwitz, ed. "Encyclopedia of Polymer Science and Technology," Third Edition, 43 pp., John Wiley & Sons, New York, DOI: 10.1002/0471440264. PST 369 (2004). Also available via: www.mrw.interscience.wiley.com/epst.

A-16: 2003 Publications (15)

538. B. Wunderlich, The Nanophase Structure of Semicrystalline Polymers and Its Influence on the Thermal and Mechanical Properties. *Proceedings of the 8th Pacific Polymer Conference in Bangkok Thailand*, Nov. 24–27, Tuesday 11/25, Plenary Lecture, 4 pages (2003).

537a M. Pyda and B. Wunderlich, Reversing and Nonreversing Heat Capacity of Poly(lactic acid) in the Glass Transition Region by Temperature-modulated Differential Scanning Calorimetry, *Proc. 31th NATAS Conf. in Albuquerque, NM*, Sept. 22–24, M. J. Rich, edt., **31,** 143/1–9 (2003).

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C: Written at Cornell University (1958–1963)*

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D: Written at Northwestern University (1955–1958)*

005. M. Dole and B. Wunderlich, Melting Points and Heats of Fusion of Polymers and Copolymers. *Makromolekulare Chemie,* **34**, 29–49 (1959).
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001. M. Dole and B. Wunderlich, The Melting Range of Semicrystalline Copolymers. II. *J. Polymer Sci.,* **24**, 139–144 (1957).
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* Look for missing numbers in later years or at the next research location. The paper number was assigned at the time the decision was made to write the paper, but its ultimate appearance depended on the time needed to complete, correct and publish the paper, which particularly for books and book chapters may have taken several years. Updated or expanded papers and new editions which are largely based on a former publication are not counted as a new publication but are identified by the letters *b*, *c*, etc. The first running index number is then identified by the letter *a*, added later.

E: Research Associates of Professor Bernhard Wunderlich during the Period 1960 to 2006

1. Postdoctoral Research Associates and Their Later Employment: (≈112 person-years)

1. Dr. Edward A. James, 1961–1962 (1 year) (British Nylon Spinners, Pontypool, Ret.).
2. Dr. Eckhard Hellmuth, 1963–1965 (2 years) (U. of Missouri, Kansas City, MO, Ret.).
3. Dr. Herbert Baur, 1963–1964 (1 year) (BASF, Ret., Ludwigshafen, Germany, Ret.).
4. Dr. Fumiyuki Hamada, 1966–1967 (1 year) (U. of Kyoto, Kyoto, Japan, Ret.).
5. Dr. M. Sansone, 1970–1971 (1 year) (Douglas Aircraft, Los Angeles, California).
6. Dr. Vera Baresova, 1970–1972 (2 years) (Weyerhaeuser Paper Co., Tacoma, WA).
7. Dr. J. Bares, 1970–1972 (2 Years) (Xerox Corp., Rochester, NY).
8. Dr. Gert Treiber, 1971–1972 (1 year) (BASF, Ludwigshafen, Germany).
9. Dr. Klaus Boehlke, 1971–1972 (1 year) (BASF, Ludwigshafen, Germany).
10. Dr. Reikichi Iwamoto, 1972–1973 (1 year) (Government Ind. Res. Lab., Ret., Osaka, Japan, Ret.).
11. Dr. Aspy Mehta, 1973–1976 (3 years) (Exxon Chemical Co., Humble, TX).
12. Dr. Maria Mucha, 1973–1974 (1 1/2 years) and 1991–1992 (1/2 year) (Technical U. of Łódź, Łódź, Poland).
13. Dr. Mark B. Altman, 1974–1976 (2 years) (Goodyear Tire and Rubber Co., Akron OH).
14. Dr. Chung Jen Lee, 1976–1977 (1 1/2 years) (Occidental Pet. Co. Grand Island, NY).
15. Dr. K. E. Weber (née Murphy), 1976–1978 (2 years) (Daemen College, Amherst, NY).
16. Dr. Rachid Benkhoucha, 1978 (1/2 year) (Algeria Industrial Service, Algeria).
17. Dr. Hua-Cheng (Peter) Shu, 1978–1979 (3/4 year) (Bayer China Co., Ltd, Hong Kong).
18. Dr. Umesh Gaur, 1979–1981 (2 years) (Textile Research Institute, Princeton, NJ).
19. Dr. Jozsef (Joe) Menczel, 1979–1980, 1985 (2 years) (Celanese, Summit, NJ).
20. Dr. Yuri Cheban, 1980–1981 (3/4 year) (Friendship University, Moscow, USSR).
21. Dr. Janusz Grebowicz, 1980–1985 (4 1/2 years) (Shell Dev. Co., Houston, TX).
22. Dr. Hidematsu Suzuki, 1982–1984 (1 1/2 years) (Nagaoka U., Japan).
23. Prof. Miao-yong Cao, 1982–1984 (2 years) (FlexoCircuits, Kingston, RI).
24. Prof. Zong-quan Wu, 1986 (1/2 year) (University of Akron, Akron OH).
25. Dr. Stephen Zheng Di Cheng, 1985–1987 (2 years) (University of Akron, Akron, OH).
26. Prof. Hai-shan Bu, 1985–1987 (2 years) (Fudan University, Shanghai China).
27. Dr. Kyriakos Loufakis, 1986–1987 (1 1/4 years) (Chemical Co., Thessaloniki, Greece).
28. Prof. Anqiu Zhang, 1987 (1/4 year, Jointly with Prof. Cheng, U. Akron, Akron, OH).
29. Dr. Manika Varma-Nair, 1988–1993 (5 years) (Exxon, Research and Eng. Clinton, NJ).
30. Dr. Yimin Jin, 1988–1993 (5 years) (General Electric, Selkirk, NY).
31. Prof. Munehisa Yasuniwa, 1988–1989 (10 months) (University of Fukuoka, Japan).
32. Dr. Bobby G. Sumpter, 1988–1992 (4 years) (ORNL, Oak Ridge, TN).
33. Dr. Alexander Xenopoulos, 1990–1993 (3 years) (Millipore Corp., Bedford, MA).
34. Dr. Nobuyuki Tanaka, 1991–1992 (10 months) (Gunma University, Kiryu City, Japan).
35. Dr. Yigang Fu, 1991–1995 (5 years) (Software Project Engineer, Palo Alto, CA).
36. Dr. Jinlong Cheng, 1992–1993 (1 year) (Emerson Electric, Murfreesboro, TN).
37. Dr. Qiguang Wang, 1992–1994 (2.5 years) (Lanzhou University, China)
38. Dr. Guanghe Liang, 1993–1994 (1 year) (Caliper Technologies Corp. Mountain View CA).
39. Dr. Marek Pyda, 1994–2006 (12 years). (Rzeszow University of Technology, Poland).
40. Dr. Stefan Kreitmeier, 1994–1996 (1.5 years) (University of Regensburg, Germany).

41. Dr. Martina Ralle, 1994–1996 (2 years) (Oregon Grad. Inst. of Science and Tech., Portland Oregon).
42. Dr. Reinhard Festag, 1995–1096 (1 year) (McKinsey and Co., Frankfurt, Germany).
43. Dr. Kazuhiko Ishikiriyama, 1995–1996 (1 year) (Toray Research Co., Otsu, Japan).
44. Dr. Iwao Okazaki, 1994–1996 (2 years, PhD conferred later in Japan, largely based on the work described in the publications listed in Part A, above) (Toray Industries, Otsu, Japan).
45. Dr. Wei Chen, 1996–1999 (3 years) (Sherwin Williams, Warrensville Heights, OH).
46. Dr. Ge Zhang, 1996–1997 (1 year) (Genaissance, New Haven CT).
47. Dr. Andreas Boller, 1996–1997 (1 year) (McKinsey and Co, Zürich, Switzerland).
48. Dr. Yon Ku Kwon, 1996–1999 (3 years) (Dept. of Polymer Science and Engineering, Inha University, Korea).
49. Dr. Il-Kwon Moon, 1997–1999 (1.5 years) (NanoSystem Lab., Suwon, South Korea).
50. Dr. Renè Androsch, 1997–1999 (1.5 years) (University of Halle, Germany).
51. Dr. Maria Laura Di Lorenzo, 1998 (9 months) (Istituto di Ricerca e Tecnologia delle Materie Plastiche, Naples, Italy).
52. Dr. Pawel Kamasa, 2000–2001 (1 year) (Research Institute for Solid State Physics and Optics Budapest, Hungary)
53. Dr. Wenbing Hu, 2000–2001 (1 year) (FOM-Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, now University of Nanjing))
54. Dr. Alexander Buzin, 2000–2002 (2 years) (Laboratory of Functional Polymer Structures, Institute of Synthetic Polymer Materials, Russian Academy of Sciences, Moscow)
55. Dr. Jeongihm Pak, 2001–2004 (3 years) (Ohio University, Athens, OH).
56. Dr. Wulin Qiu, 2004–2006 (2 years) (Georgia Inst. Technology, GA)
57. Dr. Jisheng Ma, 2004–2005 (1.5 years) (Department of Materials Engineering Monash University, Clayton Campus, 1131 Wellington Road VIC 3800, AUSTRALIA).

2. PhD Students and Their Initial Employment: (≈150 person-years)

1. Dr. David M. Bodily 1960–1964 (University of Utah, Salt Lake City, UT, Ret.) (Differential Thermal Analysis of High Polymers. The Glass Transition in Polystyrene and the Irreversible Melting of Ethylene Copolymers).
2. Dr. Tamio Arakawa 1961–1964 (Asahi Chemicals, Tokyo) (Extended-chain Polymer Crystals).
3. Dr. Peter K. Sullivan 1963–1965 (Mount Sinai Medical Center, New York, NY) (High Polymer Crystal Growth from Solution and Investigation of their Properties and Structure by Optical Interferometry).
4. Dr. Michael Jaffe 1963–1967 (Rutgers University, NJ) (The Solid State of Polyoxymethylene).
5. Dr. Theodore Davidson 1963–1967 (Consultant, Princeton, NJ) (Crystallization and Melting of Polyethylene under Pressure).
6. Dr. Frank N. Liberti 1964–1968 (G.E., Mt. Vernon, IN) (The Solid State of Nylon 6).
7. Dr. R. Bruce Prime 1965–1968 (IBM, San José, California, Ret.) (The Equilibrium Melting of Homopolymers).
8. Dr. Stephen M. Wolpert 1965–1970 (OMI OXY, Metal Ind. Corp., Madison Hts. MI) (Dynamic Differential Thermal Analysis of the Glass Transition Region).
9. Mr. Louis Melillo 1967–1972 (Pioneer Ind. Components, Springboro, OH) (Morphology of Extended Chain Crystals of Polyethylene and Polytetrafluoroethylene, incomplete).

10. Mr. Larry D. Jones 1968–1971 (Heat Capacity of High Polymers, incomplete, from the training program of the GE Co., left after passing the candidacy exam).
11. Dr. Shigeo Kubo 1968–1971 (University of Kyoto, Kyoto, Japan—deceased) (Crystallization During Polymerization of Polyparaxylylene).
12. Dr. Alexander Weitz 1969–1974 (Dow-Corning, Midland, Michigan) (The Thermal Analysis and Volume Relaxation of Glasses Formed Under Elevated Pressure).
13. Dr. Michael C. Coughlin 1969–1972 (DuPont, Wilmington, DE) (The Mechanism of Formation and the Morphology of Extended-chainCrystals of Selenium).
14. Dr. Aspy K. Mehta 1970–1973 (PD, followed by Exxon Chemical Co., Humble, Texas). (Molecular Rejection During the Crystallization of Polymers).
15. Dr. Chung Jen Lee 1972–1976 (PD, then Occidental Pet. Green Island, NY) (Polymer Crystal Growth by Crystallization During Polymerization of Diphenylsilylene).
16. Mr. George Czornyj 1970–1975 (IBM, Fishkill, NY) (Superheating During the Melting of Extended-chain and Stirrer-crystallized Polyethylene Crystals, thesis incomplete).
17. Dr. Rachid Benkhoucha 1974–1978 (Algeria Industrial Service, Algeria) (Crystallization During Polymerization of Lithium Dihydrogen Phosphate).
18. Dr. Eric Siu Wai Kong 1974–1978 (MSTI, Palo Alto, CA) (Synthesis of Extended-chain Polymer Crystals of Polydiphenylgermylene by Transport Polymerization and Crystallization During Polymerization).
19. Dr. Hua-Cheng (Peter) Shu 1974–1979 (PD, then Bayer China Co., Ltd., Hong Kong) (Selenium, Its Thermodynamic Properties and Vapor-phase Crystal Growth).
20. Dr. Umesh Gaur 1977–1979 (PD, then Textile Research Inst. Princeton, NJ) (Heat Capacities of Linear Macromolecules).
21. Dr. Suk-fai Lau 1979–1982 (Hercules, Wilmington, DE) (Heat Capacity and Thermodynamic Properties of Linear Macromolecules).
22. Dr. Richard C. Bopp, Evening student 1975–1984 (Cargill Research Laboratories, Wayzata, MN) (Differential Scanning Calorimetry of Brominated Poly(2,6-dimethyl-1,4-phenylene oxide) and its Solutions in Polystyrene, completed 5/1993).
23. Mr. Niko Gjaja, Evening student 1975–1984 (The M&P Lab Schenectady, Schenectady, NY) (Thermal Analysis of Crosslinked Systems, incomplete).
24. Dr. John P. Wesson 1978–1984 (United Technologies, Hartford, CT) (Mesophase Transitions of Polydiethylsiloxane, completed 1988).
25. Dr. Donald E. Kirkpatrick 1980–1984 (Dow Chemical, Midland, MI) (Heat Capacity, Phases, and Phase Transitions of Poly-p-xylylene).
26. Dr. Stephen Zheng Di Cheng 1982–1985 (PD, then Univ. Akron, Akron, OH) (Molecular Segregation and Nucleation of Poly(ethylene oxide) Crystallized from the Melt).
27. Dr. Lawrence H. Judovits 1980–1985 (ATOFINA, King of Prussia, PA). (The Thermal Properties of Polystyrene, Substituted Polystyrenes and Crosslinked Systems).
28. Dr. Kyriakos Loufakis 1983–1986 (next PD, then Chemical Co., Thessaloniki, Greece). (Advanced Thermal Analysis of Fluorinated and Chlorinated Polyethylenes).
29. Ms. Wonji Aycock 1984–1987 (Glenmont, NY) (Heat Capacities of Branched Polyethylenes, incomplete).
30. Dr. Robert Ya-Lin Pan 1985–1987 (Procter and Gamble, Miami, OH)(Measurement and Computation on Heat Capacities of Polyesters and other Linear Macromolecules).
31. Dr. Miao-yong Cao, 1985–1987 (before Visiting Prof.—PD, then FlexoCircuits, Kingston, RI) (The Thermal Properties of Copolymers with Anisotropic Melts).

32. Dr. Alexander Xenopoulos 1986–1990 (the PD, followed by employment with Millipore Corporation, Bedford, MA) (Thermal Analysis of Polyamides).
33. Dr. Katie A. Roles 1988–1991 (PD, followed by Macon University, Macon, GA) (Heat Capacity Study of Solid Poly(amino acid)s.
34. Dr. Jinlong Cheng 1988–1992 (then PD, Emerson Electric, TN) (Solid State ^{13}C NMR and Thermal Analysis of Conformation Motion and Disorder in Small and large Molecules).
35. Dr. Guanghe (Luke) Liang 1990–1993 (later PD, UTK/ORNL) (A Study of the Atomic Details and Dynamics of Polymethylene Crystals via Molecular Dynamics Simulation).
36 Dr. Wei Chen 1992–1996 (Later PD, then Sherwin Williams, Chicago, IL) (Characterization of the Thermotropic Mesophases by Thermal Analysis and Solid State ^{13}C NMR).
37. Dr. Ge Zhang 1994–1996 (then PD, followed by ORNL and later Genaissance, New Haven CT). (Heat Capacities of Solid State Proteins).
38. Dr. Andreas Boller, 1992–1996 (then PD, and later Mckensey and Co., Zürich, Switzerland) (The Thermal Analysis of Gel-spun Ultra-high Molar Mass Polyethylene Fibers).
39. Dr. A. Michel, 1998–1999 (1 year of a degree completed at the U. Regensburg) (University of Regensburg, Germany, under the direction of Dr. S. Kreitmeier).
40. Dr. Jeongihm Pak (2000–20001) (1 year after MS, later PD at UTK) (Reversing Melting and Crystallization of Short and Long Chain Molecules by Temperature-modulated Calorimetry).

3. Masters Degree Students and Their Initial Employment: (≈45 person-years)

1. Mr. Peter K. Sullivan 1960–1963 (Later PhD from Rensselaer) (The Interference Microscopy of Crystalline Linear High Polymers).
2. Ms. Charlotte M. Cormier 1963–1965 (IBM, Fishkill, NY) (The Effect of Extended Chain Single Crystals Seeds of Polyethylene on Crystallization from Solution and from the Melt).
3. Mr. William A. Haney 1968–1970 (Phoenix, Arizona) (Annealing of Nylon 6).
4. Mr. Aspy K. Mehta 1968–1970 (Later PhD from Rensselaer) (The Nucleation of Solution-grown Polyethylene Dendrites).
5. Mr. Arata Miyagi 1969–1971 (Bridgestone Tire Co., Tokyo, Japan) (Hydrolysis Etching and Annealing of Poly(ethylene Terephthalate).
6. Mr. Richard C. Bopp 1973–1975 (Later PhD from Rensselaer) (General Electric, Plastics Selkirk, NY) (Thermal Analysis of Poly-p-xylylene Crystallized during Polymerization).
7. Mr. Nobuhiro Toyota 1974–1976 (Sumitomo Chemical Co., Osaka, Japan) (Later PhD from Rensselaer) (Crystallization of Polyparaxylylene, incomplete).
8. Mr. Umesh Gaur 1975–1977 (Later PhD and PD at Rensselaer) (Heat Capacity Measurements by Computer Interfaced DSC).
9. Mr. Eric Siu Wai Kong 1974–1976 (Later PhD from Rensselaer) (NMR Study of the Interactions Between Nucleic Acids and Polyamines, with Dr. Bunce)
10. Mr. John P. Walsh 1977–1979 (Unknown) (Crystallization during Polymerization of a Comb-like Macromolecule involving a Mesophase).
11. Mr. Thomas M. Voll 1978–1981 (DuPont, Wilmington, DE) (The Crystallization of Single Molecule Crystals of Polyethylene).
12. Mr. Wiriya Meesiri 1979–1981 (Royal Thai Air Force Acad. Don Muang, Bangkok, Thailand) (Phase Diagram of Liquid Crystalline Polymers).
13. Ms. Jaya Pathak 1979–1981 (Pullman Kellog Co., New Jersey) (Compatibility of Polystyrene and Poly-alpha-methylstyrene blends).

14. Mr. Lawrence H. Judovits 1980–1984 (later PhD from Rensselaer) (Heat Capacity of Para-substituted Polystyrenes).
15. Ms. Mine G. Palazoglu 1982–1984 (unknown) (Studies on the Molecular Nucleation of Polymers).
16. Veronica L. Dann 1983–1985 (Abbott Laboratories, Fulton, NY) (Isothermal and Non-isothermal Crystallization of Isotactic Polypropylene: A Mesophase Crystallization Study).
17. S. Yao-Lim (Mesina) 1983–1985 (Lockheed, Palo Alto, CA) (Heat Capacities of Polyesters, no-thesis degree).
18. Robert Ya-Lin Pan 1980–1985 (Later PhD. from Rensselaer) (A Heat Capacity Addition Scheme).
19. Ms. Jeongihm Pak (1996–2000) (Later PhD. at UTK) (Melting and Crystallization of Paraffins as Model Compounds for Linear Macromolecules by Temperature-modulated Calorimetry (TMC).

4. Research Technicians and Undergraduate Assistants: (≈30 person-years)

1. Mr. J. F. Flood 1959–62 (3 years)
2. Mr. W. H. Kashdan 1960 (1/4 year)
3. Mr. D. Poland 1960–1961 (3/4 year)
4. Mr. M. L. Stahl 1962 (1/4 year)
5. Mr. A. B. DiCyan 1962 (3/4 year)
6. Mr. S. Kon 1961–1962 (3/4 year)
7. Mr. M. Jaffe, 1962–1963 (1 1/2 year) (Later PhD from RPI)
8. Mr. M. H. Kaplan 1961–1962 (3/4 year)
9. Ms. T. W. Shu 1961–1962 (3/4 year)
10. Mr. J. M. Rankin, Jr. 1964–1965 (3/4 year)
11. Mr. G. Snyder 1964–1965 (3/4 year)
12. Mr. L. Melillo 1966–1967 (3/4 year) (Later PhD student at RPI)
13. Ms. C. M. Cormier 1965–1967 (1 1/2 years) (Earlier MS from RPI)
14. Mr. C. L. Gruner 1967–1968 (1 1/2 years)
15. Mr. R. C. Bopp 1968–1973 (4 1/2 years) (Later MS and PhD from RPI)
16. Mr. G. Czornyj 1969–1970 (3/4 year) (Later PhD student at RPI)
17. Ms. B. A. Dean 1972–1973 (3/4 year)
18. Ms. C. C. Wunderlich 1976 (1/4 year)
19. Mr. B. B. Wunderlich 1977–1980 (1/2 year)
20. Mr. J. Berninger 1980–1981 (1 year)
21. Ms. K. Wilson 1983–1984 (1 year)
22. Mr. J. R. Reffner 1983–1985 (2 years)
23. Ms. J. Woertman 1986–1987 (1 year)
24. Mr. R. Jones 1988–1989 (1 year).
25. Ms. S. Gerdes 1992–1993 (1 year).
26. Ms. M. Ribeiro 1996 (1/4 year).
27. Ms. Pia Van Bentham 2001 (1 year)
28. Mrs. E. Nowak-Pyda 2003–2006 (2 years).

Totals: ≈340 person-years, 144 persons. (The time-average for completion of a PhD ≈4.0 years).

Appendix B

Thermal Analysis of Macromolecules

ABSTRACT This Appendix contains a personal review, tracing the development of thermal analysis as experienced and contributed to by the author. The article touches upon the beginning of calorimetry and differential thermal analysis (DTA) for polymers, the development of *dynamic differential thermal analysis (DDTA)*, differential scanning calorimetry (DSC), *single-run DSC*, up to the more recent additions of temperature-modulation to DSC (TMDSC), and the accomplishment of super-fast calorimetry. New words and phrases were introduced, leaving a trail of the developing research. First, there was the observation of *cold crystallization* in my PhD thesis research in Professor Dole's laboratory in 1955–1957. This was followed by attempts to understand polymer crystals through their *irreversible thermodynamics of melting* by investigation of zero-entropy-production melting, and the glasses with DDTA, in support of the rule of *constant increase of C_p at the glass transition* per mobile bead in flexible molecules. Most recently, the terms *decoupled chain segments in nano phases* and *glass transitions of crystals*, were coined. In-between, the *Advanced THermal Analysis System*, *ATHAS*, was created and the phenomena studied were: *extended-chain crystals*, *crystallization during polymerization*, the *chain-folding principle*, *single-molecule single-crystals*, *molecular nucleation*, *condis crystal*, and *oriented intermediate phases*. Melting kinetics and *superheating of polymer crystals* were analyzed, *amorphous defects* and *rigid-amorphous phases (RAF)* discovered. All this led gradually to a new *system of classifying molecules*, their *macroconformations* and *phases*. The *rules for entropy of fusion based on molecular shape and flexibility* and definitions for *macro*, *micro*, *and nano phases*, helped to understand *the globally metastable*, *semicrystalline polymers* which may contain local subsystems which *melt reversibly.*

A. INTRODUCTION

It was a special honor to be asked to add a personal review of 'Thermal Analysis of Macromolecules'in recognition of my 75th birthday to the special symposium issue of the *Proceedings of the 34th NATAS Conference*. At the same time, this is also the 60th anniversary of my interest in Chemistry and the 50th anniversary of the beginning of my work in thermal analysis and polymer science. It is amazing how fast time passes when one has fun with what one is doing.[1]

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[1] This review is written based on an earlier publication of 1996 on the occasion of my 65th birthday, published in the *J. Thermal Analysis*, **46**, 643–680 (1996) (see pages 9-18 and 52). It appeared later in an updated form in the *Proc. 34th NATAS Conf.* in Bowling Green, KY, Aug. 6–9, 2006, and in the *J. Thermal Anal. Cal.,* **89**, 321–356 (2007). The present reworking as Appendix B, removes any duplications with the body of the book, and extends the research discussions to the year 2010.

In 1946, I discovered chemistry by reading the 2nd edition of K. A. Hofmann's 'Inorganic Chemistry' of 1919. The year before, the book had ended up in my collection when the two floors of our apartment building collapsed during the bombing (see Chapter 2, Figure 9). The downstairs tenant used it in his studies and thought I might enjoy it. What an enormous source of interesting facts and historical footnotes! In 1947, chemistry was introduced as a high-school subject, and being properly primed, I advanced in this subject quickly to the top of the class. Ultimately, I chose chemistry for my university study in 1949. At the University of Berlin (Humboldt University, 1949–53) I could use the same book for my basic study. The 14th edition edited by U. Hofmann (and Ruedorf) of 1951 is still on my book shelf and, over the years, has answered many questions. The early period of my study in chemistry is treated in more detail in Chapters 3 and 4.

The beginning of the university study was not without problems, as mentioned in Chapter 4. It took the forceful intervention of Professor E. Thilo of the Humboldt University to overcome the problem of my not belonging to the preferred class of workers and peasants and not being properly politically active. Besides teaching me how to teach chemistry, Professor Thilo also instilled an interest in phosphates and silicates. Many years later, a student of mine and I could contribute some new knowledge about *crystallization during polymerization* of LiH_2PO_4, using thermogravimetry (TGA) and differential scanning calorimetry (DSC) [1].

My graduate education began as Research Assistant to Prof. Malcolm Dole at Northwestern University in Evanston, IL. The subject of study was calorimetry of polymers. It was a very opportune time for this topic. 'Polymers' were still a relatively new subject, taught at very few universities, and calorimetry has always been a topic for only a few, select researchers. Professor Dole, being a former coworker in Professor Debye's Institute in Leipzig, Germany, in 1929, and having gained interest in polymers already before WW II, was the unique expert in the field to educate students [2]. Under his expert guidance, it (only) took until 1957 to complete my PhD thesis on the 'Thermodynamics of the Copolymer System Poly(ethylene terephthalate-*co*-sebacate)' [3, 4]. Besides heat capacity measurements, the process of *cold crystallization* was recognized and named. This process occurs somewhat above the glass transition temperature and is the limiting nonequilibrium mode of crystallization. During a subsequent year, as instructor at Northwestern University, the kinetics, thermodynamics, and statistics of this nonequilibrium crystallization and melting was analyzed with help of the, at that time, revolutionary and brand new electronic calculator (IBM 650, see page 6-33) [5]. Figure 1 illustrates the broad area of possible nonequilibrium crystallinity in copolymers of polyterephthalates, using the experiment-backed assumption that cold crystallization is limited to nanocrystals of three repeating units in length (≈3 nanometers). Chapter 6 deals in more details with this early time in my developing research interests.

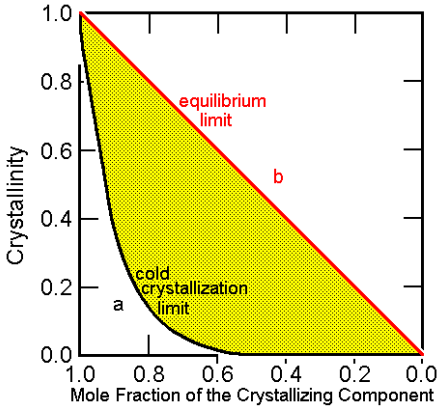

Figure 1 *Mass fraction crystallinity, w_c, of A in poly(A-co-B) after cold crystallization as function concentration. Curve a is the lower limit of nonequilibrium crystallinity. Curve b indicates the equilibrium crystallinity [5].*

Many of the present research topics of our *Advanced THermal Analysis System*, *ATHAS*, have their roots in this first look at the thermal properties of polymers. This early work was extended at the Department of Chemistry at Cornell University from 1958 to 1963, where I was an instructor, and later assistant professor, (see Chapter 7, and Sect. B, below). The main direction of my research was then generated during the almost 25 years tenure at Rensselaer Polytechnic Institute (1963–88) as Professor of Chemistry (promotion to full professor in 1965, see Chapter 8, and Sects. C, and D, below). After early retirement from RPI, the next stage of research was begun at The University of Tennessee and at Oak Ridge National Laboratory (1988–2001). This work is covered in Chapter 9 of the book, and Sects. E and F, below. After final retirement, some work was continued by building on the prior experience (see Chapter 10 and Sects. G and H, below). The idea of the *ATHAS* was finalized in March 1980. Ever since, it has been the focus of the research of my students and postdoctoral fellows. The ATHAS Laboratory, finally, was moved to the Department of Chemistry at the University of Technology in Rzeszow, Poland by Dr. Marek Pyda who was from 2001–2006 Director of the ATHAS Laboratory (see also pages 10-5–7). It is hoped that by this move, the ATHAS information will remain available to the thermal analysis community and grow for the benefit of everyone. In Chapters 1–4 of the book many early personal details are added, in Capters 5–10 the later aspects of my life and descriptions of the general growth of the laboratories at the different universities are added to the scientific developments given here in more detail.

B. EARLY CALORIMETRY AND KNOWLEDGE ABOUT SOLID POLYMERS (1955–1965)

Most calorimetry on polymers in this early time period was done by adiabatic calorimetry. The instrumentation was based on the classical design of Nernst [6]. Major calorimeters were only in operation at the Bureau of Standards [7] (now NIST) and in Prof. Dole's laboratory [8] (see Chapter 6, Figure 18). During this decade these two major producers of data on polymers were joined by the GE Research Laboratory (Karasz *et al*. [9]) and work was begun at the University of Leeds, England (Dainton, *et al*. [10]). A check of the literature [11] revealed that through 1955 only 30 papers on heat capacity of linear macromolecules were published, describing mainly natural and synthetic rubbers, polystyrene, poly(vinyl chloride), polyethylene, selenium, nylon 6, poly(tetrafluoroethylene), and poly(fluorotrichloroethylene). The first papers on heat capacity of characterized polymers date back to 1928 [12], 1935 [13], 1937 [14] and 1938 [15]. The basis of the theory of heat capacity of solids was given by Einstein [16] and Debye [17], and an extension to polymers was suggested by Tarasov [18]. A detailed analysis of the vibrational characteristics of a polymer was attempted by Stockmayer and Hecht [19]. This means, by 1955 a solid foundation existed for research about the thermal properties of polymers. The two major limitations were that most attempts to understand the thermal properties of macromolecules made use of an equilibrium approach, and that the morphology of crystalline polymer crystals and their molecular link to the surrounding amorphous fraction was not well understood.

The knowledge of flexible macromolecules in the solid state underwent a dramatic change in the following years. Polymers with rather regular chemical structure were known to crystallize, but only partially. Less regular polymers were glassy at sufficiently low temperature. Both states of matter are not in equilibrium. With the help of electron microscopy it could be shown in 1955–60 by Keller, Fischer, Till, Geil, and Kobayashi that flexible macromolecules are prone to crystallize in a lamellar morphology [20, 21]. The polymer molecules are much longer than the lamellae are

thick and fold or leave the crystal phase at the lamellar surface. The lamellar thickness (fold length) was found to be 5–50 nm, making the crystals highly metastable. Optical interference microscopy [22] was developed in our laboratory for quantitative analysis of the morphology and measurement of lamellar thickness [23]. Extending the measurements on polyethylene to solution-grown single crystals produced at pressures up to 600 MPa gave proof that the reason for chain folding was kinetic and not thermodynamic. By covering a 100-K range of crystallization temperatures, the lamellar thickness was found to change with super-cooling and not with temperature [24].

The experience with crystallization under elevated pressure led to the discovery of *extended chain crystals* of polyethylene [25]. At pressures above about 300 MPa, linear polyethylene melts would, after crystallization to folded-chain lamellae, anneal to a thickness that could reach the molecular lengths of typically 1–10 μm and also achieve close to 100% crystallinity. These observations meant that, given the right experimental conditions, the whole spectrum from the common, metastable *macroconformation* in folded-chain crystals to the *extended-chain*, equilibrium crystals could be produced and was in need to be studied by thermal analysis.

For thermal analysis, it was necessary to learn how to deal with the metastability of solid polymers. As the melting point is approached, annealing, reorganization and recrystallization to higher stability is possible, i.e., the sample may change during calorimetry. The first solutions were to run calorimeters as fast as possible and avoid the intermittent stops to regain temperature equilibrium [26, 27]. The next step was to build new calorimeters for smaller masses, adapted to continuous and faster heating [28]. Finally, in 1960, continuous differential calorimetry for masses as little as one gram, and with heating rates as fast as 1.0 K min^{-1} was demonstrated by Müller and Martin [29]. Soon thereafter, two radically new commercial calorimeters were introduced, the differential scanning calorimeters (DSC) by the Perkin-Elmer Corp. Norwalk, CT, [30] and by the DuPont Instrument Division, Wilmington DE (now TA Instruments, Inc.). These instruments permitted quantitative measurements for masses of 10 mg and with heating rates as fast as 40 K min^{-1}. Such DSCs are today's principal tools for the analysis of metastable and unstable states.

Before the development of commercial DSCs, we adapted differential thermal analysis, DTA, to the measurement of heat (calorimetry) [31], as we had adapted before adiabatic calorimetry to continuously measure heat [26]. For the first time, it became possible to show by thermal analysis that the unusually large specific surface free energy of the thin lamellar crystals of polyethylene can cause a substantial decrease in melting temperature [31]. It could also be proven that the fold surfaces introduced additional, and often the major melting point lowering in copolymers [32]. This insight into the *irreversible thermodynamics of melting* of polymer crystals was summarized in two basic papers on defect polymer crystals. The papers were published in England because of referees who did not grasp the importance of nonequilibrium processes [33] (see pages 7-19–20). A path of zero-entropy-production melting using fast heating was proposed, contrasting the commonly accepted slow heating. The rationale was to achieve a quick transition from the metastable crystal to an equally metastable melt. Slow heating brings changes in perfection of the crystals and may suggest erroneously high melting points for the starting material. For random copolymers, slow melting has some use. It can detect the last crystals that dissolve into the melt. The melt has then the concentration which was set by the synthesis of the copolymer. The last crystals melting, thus, see no concentration changes that are caused by segregation on crystallization.

The other metastable state, the glass, was also analyzed in our laboratory. A special, sequential heating and cooling method was invented, a method called *dynamic differential thermal*

analysis, or *DDTA* [34]. The kinetics of the freezing of polystyrene was derived mathematically [35] and compared to the DDTA experiments, using the hole model of the liquid state, as applied to polymers by Hirai and Eyring [36]. It could be demonstrated that the glass transition temperature, T_g, changes logarithmically with cooling rate, and that the hysteresis (enthalpy relaxation) can be described mathematically. The rather cumbersome equations could be handled with the help of an electronic computer. Studying all available calorimetric data on the change of the heat capacity, C_p, at T_g allowed us to formulate the rule of *constant increase of C_p at the glass transition temperature* per mobile bead within the molecule [37]. This rule states that every flexible part of a molecule (bead), has a heat capacity increase of about 11 J [K (mol of beads)]$^{-1}$. It permits the estimation of the flexibility of a molecule by thermal analysis, and also documents that the change in heat capacity at the glass transition temperature is an extensive thermodynamic quantity and can be used to find the amount of amorphous material in a multi-phase material.

To understand a metastable state, the equilibrium state must be well characterized since it forms the limit to which the metastability must be compared. Heat capacities are the basis of all thermal properties and most important for such characterization. The total heat content, H, is not measurable directly. It must be calculated by summation of the measured incremental amounts of heat capacity, $C_p = (\partial H/\partial T)_{p,n}$, (the heat added per kelvin at constant pressure, p, and constant composition, n):

$$H(T) = H(T_o) + \int_{T_o}^{T} C_p \, dT \qquad \textbf{(1)}$$

This equation underscores the importance of either measuring the heat capacity over the whole temperature range, or to develop a theory that allows extrapolations of incomplete data. The latter approach was taken in our laboratory for the evaluation of the heat capacity of solids (glasses and crystals, see Section H). For liquids, it is necessary to establish data over wide enough temperature ranges to safely extrapolate beyond the experimentally accessible temperature range. In case chemical reactions or physical changes occur within the sample during the calorimetry, their latent heat, $L = (\partial H/\partial n)_{p,T}$, must be added separately to Eq. (1). The latent heats evolved or absorbed do not change the temperature and are to be measured as a function of the changing composition, n, at constant pressure, p, and temperature, T. If, however, the analyzed system described in Eq. (1) responds slowly to the change in temperature, the rate of measuring must be slowed also. To remain in equilibrium, the rate-of-measuring must be such to complete all processes. Another mode of measurement is to bypass the changes completely by sufficiently fast measurement. For C_p measurements, a slow response is expected in the glass transition region. During measurements of latent heats, chemical reactions and processes of ordering and disordering might be slow.

In the solid state, the heat capacity consists almost entirely of vibrational energy. Based on the work by Einstein [16], Debye [17], and Tarasov [18], an approximate vibrational spectrum was fitted by us to the heat capacities that are often only known over a limited temperature range. Polyethylene (PE) was the first fully analyzed sample [38]. The experimental heat capacities [26] were combined with all literature values to a data bank that could be extrapolated to 100% crystallinity, as shown in Figure 2. The limiting, extrapolated heat capacities are given in Figure 3. The fit to the approximate frequency spectrum consisting of skeletal and group vibrations is shown in its later, final form in Figure 4 [39]. For the first time, the measured equilibrium thermal properties could be linked to a vibrational spectrum to understand the motion in the solid state of macromolecules [40]. It was then also possible to give quantitative information on the degree of

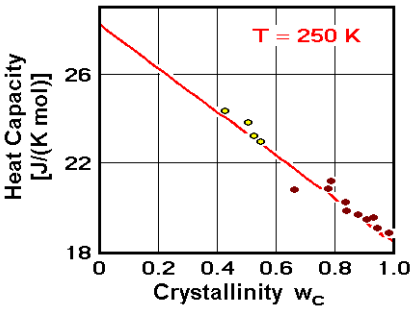

Figure 2 *Extrapolation of the measured C_p to the crystalline and glassy PE. Filled circles refer to linear PE, open circles to branched.*

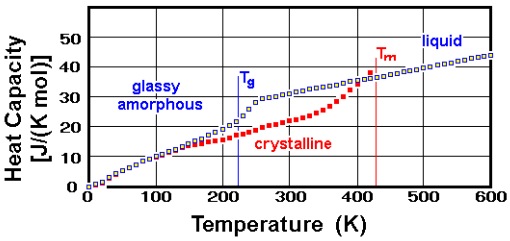

Figure 3 *Heat capacity limits for liquid and crystalline PE as can be gained from extrapolation of data as shown in Figure 2. Note the broad glass transition.*

order of the crystals via the entropy *S*, and the stability, via the free enthalpy *G*. Figure 5 displays the result. This first analysis led to similar results for over 200 polymers and polymer-related materials of low molar mass in the ATHAS Data Bank (see pages B-13–16, 21–22, 34, 41 [83]).

Figure 3 also displays the heat capacity of the amorphous state (crystallinity = 0% in Figure 2). At high temperature, this refers to the melt, at low temperature to the solid (glass). The glassy state is quite difficult to reach for the fast crystallizing polyethylene, but Figure 3 displays clearly a glass-transition temperature of 237 K. Of special interest is also the rather gradual beginning of the glass transition, starting at about 120 K. This was explained as a slow beginning of local conformational motion involving the gauche-trans equilibrium of the backbone C–C-bonds. Data were gained from estimates of the conformational energy by interpretation of mechanical properties and the measurements of mobility by solid state NMR [41].

These first ten years of research in polymer morphology and thermal properties confirmed the value of full analyses of materials using structure and energy considerations. It became clear that the two roots of the full description of materials are their mass and energy. Quantitative methods for the measurement of mass and energy were equally well developed at the beginning of modern science, some 200 years ago [42]. Based on the constancy of combining ratios of the masses of elements in chemical reactions, Dalton [43] could prove the atomic theory of matter. This started developments that today lets us 'see' molecules in full structural detail. The magnification factor to go from the

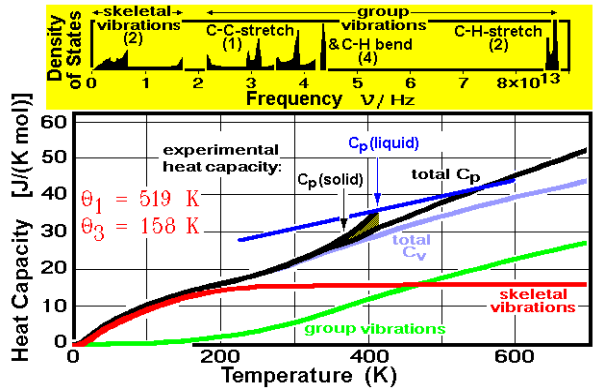

Figure 4 *Contributions to the heat capacity of polyethylene.*

atomic scale (0.1 nm or 1 Å) to the macroscopically visible scale (1 μm) is 10^4. While the research into the mass of matter took now a path to find more and more structural detail on an atomic, microscopic level, the research into the energetics went in the direction of the macroscopic description through thermodynamics [44]. Its link to the molecular motion was limited largely to the description of ideal gasses ($pV = nRT = ⅓ M\overline{v^2}$, where $\overline{v^2}$ is the mean square particle velocity). The reason for this preference of the macroscopic description of energetics is the large scaling factor needed in 'visualizing' molecular motion in the various condensed states. It became only possible through simulation of crystals on supercomputers to 'see the molecular motion [45] (see Section E). The molecular time scale for large-amplitude motion is in the picosecond range (10^{-12} s). A comparison to the fastest observable processes by the human eye, at best, one millisecond (10^{-3} s), needs a scaling factor of 10^9! This is much further removed from the macroscopic experience than structure information and may be the reason why the link of molecular motion to thermal and mechanical properties is only now developing (see pages 9-14–17, 42–48).

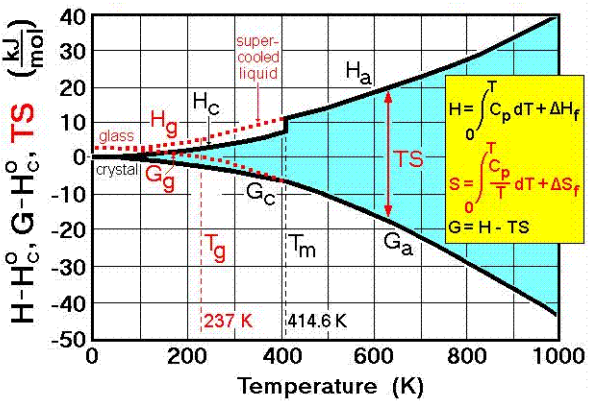

Figure 5 *Thermal properties of polyethylene: enthalpy, H, free enthalpy, G, and entropy S (as TS). The subscripts are:* 'a' *for amorphous,* 'g' *for glass, and* 'c' *for crystal. The link to the experimental heat capacities is established by the equations in the insert, glass transition and melting transition are marked.*

C. FIRST WORK ON DSC & STRUCTURE AND MORPHOLOGY OF CRYSTALS (1965–1975)

Into the early 1960s falls the availability of commercial DSC equipment that was far superior to any self-built instruments. We bought our first Perkin-Elmer DSC-1 in 1965. Within a few days I could extend the earlier measurements on semicrystalline polyethylene, discussed in Section B, to equilibrium crystals of polyethylene [46]. Completely crystalline and extended-chain samples were available by then [25]. The quality of the new data rivaled even those we could gain by adiabatic calorimetry [26]. Coupled with dilatometry, the equilibrium melting temperature, T_m°, could be fixed within a fraction of a kelvin to be 414.6 K, and the difference between equilibrium and nonequilibrium dissolution temperatures could be used to estimate the surface free energy γ (0.083 J m^{-2}) by using the Gibbs-Thomson equation [47], and structural data from low angle X-ray diffraction, electron microscopy [21], or optical interference microscopy [23]:

$$\Delta T = \frac{2\gamma T_m^\circ}{\Delta h_f \rho l} \qquad (2)$$

where Δh_f is the heat of fusion (293 J g^{-1}), ρ, the density (1.0 Mg m^{-3}), and l the lamellar thickness. A lamella of 10 nm thickness has a specific surface area of 200 m^2 g^{-1} and leads to a ΔT of 23.5 K. The enormous surface areas of polymer crystals explain most of their metastability. This straightforward experimentation revealed two additional important facts. First, the heat capacity of polyethylene is what one would expect from extrapolation of paraffin data. Later research detailed that a continuous change in C_p with chain length occurs at very low temperatures. It starts with solid hexane and is due to a steady increase in the intramolecular skeletal vibration frequencies (Θ_3) [48]. Second, extended-chain crystals melt rather slowly and can lead to *superheating of polymer crystals*, i.e., melting is slower than the conduction of the heat of fusion into the sample [49]. A new field of study was initiated, the kinetics of melting, to be contrasted to the kinetics of crystallization. This topic was also our contribution to the First and Second International Congresses on Thermal Analysis (ICTA) at Aberdeen, Scotland and Worcester, MA in 1965 and 1968, respectively [50] (see page 8-23). In Aberdeen, our contribution in the field of polymer science was one of five presented (131 papers, overall). Things have changed over the years, polymer science is by now the main user of thermal analysis. This is chiefly due to the good precision of DSC and its easy availability.

The about 100 publications that were generated from 1965 to 1975 at RPI can be summarized in six major topics, to be discussed next with key citations: 1.) Continued work on *extended-chain crystals* [51]. 2.) *Crystallization during polymerization*, a topic that arose directly out of the effort to understand the chain folding [52]. 3.) *Molecular nucleation*, a result which grew out of topics 1 and 2 [53]. 4.) Continued analysis of other polymers besides polyethylene. 5.) The glass transition of pressure-densified polymers. 6.) Creating books and book chapters to describe the newly gained knowledge and fit it into the prior understanding [11, 21, 54] and also teaching the field with a new method, that of the Audio Course [55]. All throughout, thermal analysis was providing the direction for new research and was also central to in develop better understanding of polymer science.

The knowledge gained on extended-chain crystals [51] was the key to the understanding of metastability in polymer crystals, with polyethylene being the model for flexible macromolecules. We originally thought seeding with equilibrium crystals might help in growing more stable crystals, but it just is not so [56]. Thermal analysis showed that there is only little enhancement of crystallization due to the presence of even the most perfect nucleating agents. It was also shown in this research that folded chain crystals are initially less perfect and subsequently anneal at the crystallization temperature to a more perfect state. The first steps of crystallization yield lower-melting crystals. These observations suggest limits to the classical theory of polymer crystal growth which is based on single-step addition of segments that span the full lamellar thickness [21, Vol. 2]. Morphological details of the nucleation, growth, annealing, and melting were generated by electron microscopy [57, 58]. The observed nuclei of crystals growing on an extended-chain crystal-surface bypassed the available secondary nucleation sites. Locations of secondary nuclei were ignored by the molecules, pointing to other reasons hindering crystal growth. Experiments on polypropylene and computer simulations led Binsbergen to quite similar conclusions [59]. Secondary nucleation does not govern the rate of crystallization.

The mechanism of chain extension on crystallization of polyethylene under elevated pressure provided another puzzle. From the microscopy of the crystals and the thermal analysis of melting, it was clear that the initial crystal had to be chain-folded [51]. The chain extension had to be a subsequent annealing step [58]. Why, however, does the more restrictive crystallization under high pressure permit chain extension? This question was resolved in two stages. First, Bassett observed

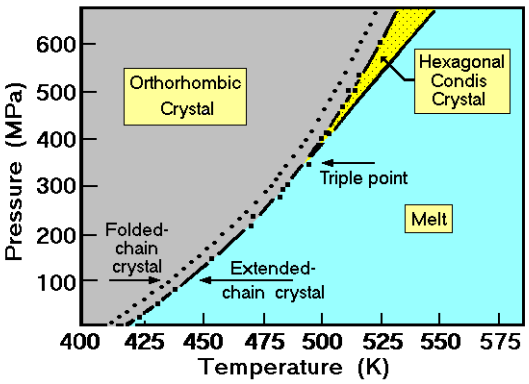

Figure 6 *Phase diagram of polyethylene.*

in 1972 that at elevated pressures, a hexagonal phase is stable [60]. The corresponding phase diagram is shown in Figure 6. We could later identify this new hexagonal crystal phase as being conformationally disordered, i.e., representing a *condis crystal* [61]. Only condis crystals have the required high mobility for fast diffusion of the chains through the crystal for full chain extension. Although not all flexible polymers that crystallize as a condis phase anneal to extended-chain crystals, all the extended-chain crystals grown from the polymer melt were at least initially condis crystals [62]. Pressure, in turn, is not a prerequisite. Examples, of extended chain crystals which can grow at atmospheric pressure are poly(tetrafluoroethylene), poly(chlorotrifluoroethylene), poly(diethylsiloxane), *trans*-1,4-polybutadiene, and poly(diethyl siloxane).

Having observed initial chain folding even for crystals perfected to extended-chain crystals, I felt certain that one can formulate a *chain-folding principle* [21, Vol. 1, p. 193]: "A sufficiently regular, flexible linear macromolecule crystallized from the mobile, random state will always crystallize first in a chain-folded *macroconformation*." This chain-folding principle has naturally a corollary: It should be possible to grow extended chain crystals directly on *crystallization during polymerization*, bypassing the polymeric, random state. My first sabbatical leave 1966/67 (see pages 8-37–48) at the University of Mainz was used to investigate this question [52]. Many indications that extended chain crystals of polymers can grow from the monomer were already in the literature, and a further series of examples was analyzed by us in the following years (selenium from the vapor [51, papers VII and IX], poly(oxymethylene) from trioxane [63], polyparaxylylene from the cyclic paraxylylene dimer [64], polyethylene from diazomethane [65], lithium polyphosphate from the lithium dihydrogen phosphate [1], and poly(tetrafluoroethylene) from the gaseous fluoroethylene [51, VIII]. For more details see [21, Vol. 2]. Figure 7 shows the schematic of extended chain crys-

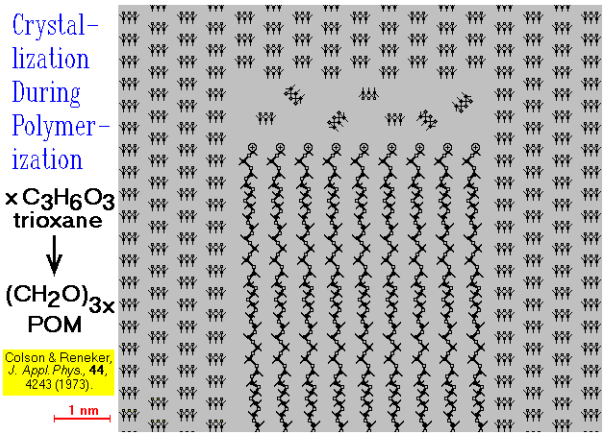

Figure 7 *Schematic of crystallization of poly(oxymethylene) during polymerization from trioxane crystals.*

tal growth of poly(oxymethylene) inside a single crystal of trioxane. Similar simple mechanisms can often lead to fully extended equilibrium crystals of flexible macromolecules. A large number of intermediate cases have also been identified where crystallization occurs shortly after polymerization. In these cases, the degree of chain folding is an indicator of the flexibility of the polymer and the separation in location and time of the polymerization and crystallization site. This turned out to be specially important for the discussion of biological syntheses, as exemplified by celluloses and silks [21, 52]. The crystallization during polymerization provides also the bridge to knowledge of crystallization of small molecules.

It was suggested above that secondary nucleation was not the rate-determining step in crystallization of flexible polymers. If it is not, what takes its place? The crystallization kinetics of all analyzed flexible polymers had shown an exponential crystallization rate, dependent on the inverse of the supercooling, a clear sign of some type of nucleation control [21]. This seeming contradiction is not yet fully resolved, but a qualitative discussion can be given as follows: Plots of melting and crystallization rates *versus* temperature exhibit breaks, as shown in Figure 8. The kinetics is not continuous through the equilibrium melting temperature, in contrast to the Onsager principle of microscopic reversibility. There is a region of metastability below the equilibrium melting temperature where the melt is metastable. Even seeding with stable crystals does not break this metastability [56]. In addition, our study of crystallization indicated that a growing crystal in a melt consisting of a broad distribution of molar masses can reject molecules of sizes that could grow to stable crystals. This segregation is close to perfect and must have a reversible step [66]. Our suggestion was that there must be a *molecular nucleation* step [53, 66]. The molecular nucleus involves all or a portion of the molecule as a first step of crystallization. The molecular nucleation provides, thus, the rate-limiting step and depends on the degree of supercooling [21]. It also explains the rate dependence of crystal growth, as illustrated in Figure 8, the molecular mass segregation and, furthermore, satisfies the irreversibility of crystallization and melting. The irreversibility is now moved to the level of a single or part of a molecule. Once a molecular nucleus exists, the crystal can *melt reversibly* on a local sub-molecular scale. If the molecule is completely removed from the crystal surface, new molecular nucleation is required with the necessary supercooling, explaining the break in Figure 8. Although a quantitative description of molecular nucleation is still outstanding, all of the many experimental results seem to be in qualitative agreement with the molecular nucleation concept. Besides the model polyethylene [53, 66] an even more complete analysis was carried out later on poly(oxyethylene)s [67]. More recently, dynamic Monte Carlo simulation was applied to crystallization by Prof. W. Hu, and, indeed, showed evidence of an intramolecular nucleation [68].

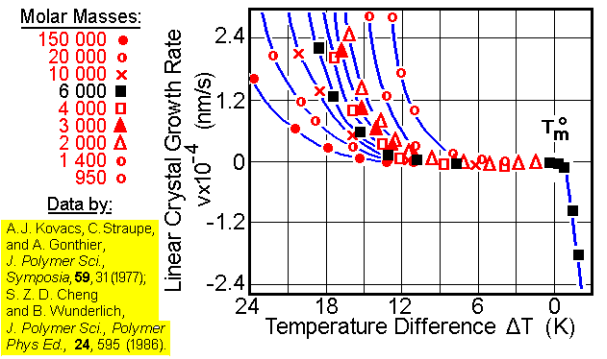

Figure 8 *Illustration of the break between crystallization and melting rates for poly(oxyethylene)s of different molar mass.*

The detailed thermal analysis beyond polyethylene began with poly(oxymethylene) [63]. Observed could be superheating, double and multiple melting peaks, crystal perfection on heating, recrystallization, annealing, and ultimately, decomposition. General free enthalpy diagrams were derived that permit to visualize the metastable states and their transitions, as shown in Figure 9. All of the indicated transitions in Figure 9 could be documented and their special signature in thermal analysis was identified. Other polymers studied included poly(ethylene terephthalate), of interest because of its ease of change of the backbone structure through etching and solid state polymerization [69]; selenium, a polymer that can open its folds to anneal to extended chain crystals [70]; polyparaxylylene, that shows several polymorphs and can be crystallized during or immediately after crystallization [71]; polycaprolactam (nylon 6) that can also be polymerized into the solid state [72]; and poly(tetrafluoroethylene), a molecule with an intriguing polymorphism [73]. Another set of compounds that caught our interest were the tetraalkyl ammonium salts [74]. More will have to be said below about these tetraalkyl ammonium salts and other small, flexible molecules and their mesophases.

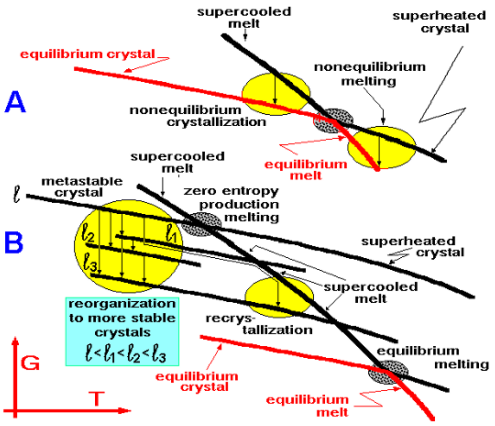

Figure 9A, B *Two free enthalpy diagrams to correlate the (A) equilibrium and (B) nonequilibrium states of typical polymer crystals: Annealing, reorganization, recrystallization, crystallization, and melting. Upward transitions between the states are forbidden by the second law ($\Delta G \leq 0$ for transitions).*

The work on glass transitions was continued with a study of the hysteresis for glucose, selenium, poly(vinyl chloride), polystyrene, poly(methyl methacrylate), and poly(oxy-2,6-dimethyl-1,4-phenylene) (PPO) [75]. The parameters for kinetic descriptions [35] were determined. Low-molar-mass and high-molar-mass compounds behaved similarly. What was not expected was that densified glasses obtained on vitrification under elevated pressure did not have a lower enthalpy. On annealing, they showed a relaxation with different relaxation times for dilatometry and calorimetry [76]. This precludes a description of the glass transition as processes governed solely by free-volume or entropy concepts, as is frequently suggested in an effort to reach a simple description. Another concept, that of tie molecules or decoupled chain segments of molecules residing in different crystals were known from electron microscopy [21] and their presence could be proven by DSC [77]. Its importance was understood much later and is discussed in Sect. G.

The new information had to be fitted into the overall picture. Two special leaves were spent in the library to write the treatise 'Macromolecular Physics' [21] (see the pages 8-57–58 and 62–63). Flexible macromolecules were placed into a system for *classifying molecules*, as shown in Figure 10. Another clarification introduced was the nomenclature for the overall shape of a flexible macromolecule: The *macroconformation*. The term macroconformation is distinct from the terms conformation which describes the limited arrangement about one or several bonds (also called rotational isomerism) and morphology, which describes the shape of a crystal consisting of many molecules. The macroconformations of polymers are identified in Figure 11.

The summary of the emerging knowledge about defects of polymers as described in [21, Vol. 1] led to the introduction of the idea of *amorphous defects*. An amorphous defect is a three-dimensional defect, caused by molecules that are partially included in the crystal. It is thus a phase, but of nanometer size. Initially, the amorphous defects could be assessed through the decrease in crystallinity, but they must be tied intimately to the crystal, since the bulk-amorphous phase can crystallize, the amorphous defects do not. Together with the chain folds, they are the major causes of metastability in the polymer crystals. Later research built on these initial observations as seen in Sects. F and G.

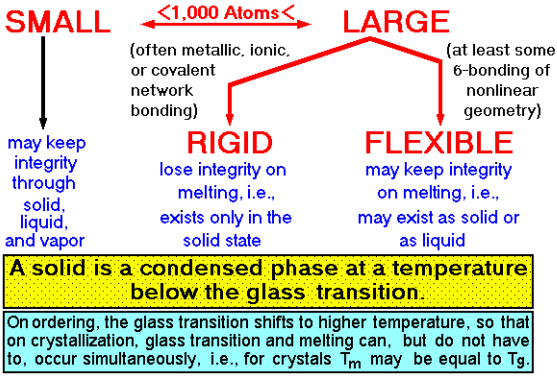

Figure 10 *Summary of all types of molecules.*

Increasingly troublesome proved that the object of my specialization, polymer science and thermal analysis, could not draw enough students within most universities to justify a full-time teaching effort. This does not mean that I did not enjoy teaching freshman chemistry, but I felt that the unique knowledge that was accumulated over the years of research could not be taught in proportion to its potential value to science and industry. An experiment was made with developing of audio courses [55]. Special, condensed lectures were recorded for the audio courses and combined with books of summaries and blackboard material. Each of the courses was equivalent to one semester of three credit hours. Although not the same as live lectures, the audio courses provided detailed instruction to anyone interested, independent of teaching schedules and location. They also were of value to the increasing number of graduate students with English as their second language. At RPI, the Evening Division handled the student registration, and I arranged for up to six hours of personal tutoring, exams, and grading through oral exams. The courses ran cost effective. Indeed, it would have been possible to reduce the tuition from the high private-school level and still be profitable. More than

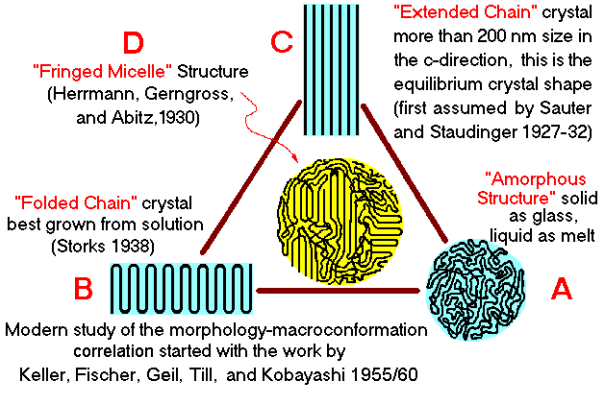

Figure 11 *Molecular macroconformations that describe the shape of polymer molecules within crystals, melts, and glasses.*

200 students went through these audio courses at various locations. It opened the possibility for a professor to teach simultaneously at several universities and/or companies. The local organization would provide the students interested in the subject, schedule occasional personal visits by the author, and if needed, run tutorials and schedule exams. The experiments showed that the method works, but universities (and professors) are still too conservative to underwrite such changes in teaching methods with their wide-ranging implications (see also the pages 8-66–75 and 9-35–37 for a more detailed discussion of problems of teaching and methods to solve them).

D. COMPUTERIZATION AND FORMAL DEVELOPMENT OF ATHAS (1975–1988)

The time period of this Section brought a special advance in thermal analysis. Computers were added to DSC for data acquisition, treatment, and ultimately analysis and storage (data banks). In our laboratory, the modification began with adding electronic calculators with a tape or card-punch for mass data storage [78]. Next, we found that expert help from computer programmers was necessary to design a fast computer that could do both, acquisition and calculation of data [79]. Later, the manufacturers introduced their own, proprietary software. This latter development may have hampered independent programmers to create the specialized, more transparent software that is needed for many scientific applications. In a workshop at the 8th ICTA in Bratislava (1985) this problem was discussed and suggestions were made, but largely ignored by all manufacturers of DSCs [80]. Today, it is still not easy to link the DSC output directly to data banks, thermodynamic function generators, and independently developed or acquired mathematics packages.

The introduction of affordable personal computers of the Apple, Atari, and Commodore trademarks in the late 1970s and early 1980s did not only provide entertainment with games. These 'personal computers' of only 32–64 kB of RAM were also suited to produce sound and pictures for instruction in the form of computer courses [81] (see pages 8-69–71). For about 20 years, these programs ran on the old computer in our laboratory. They included lectures, exercises, and exams. Modern computers are dominated by the not so teaching-friendly Microsoft programming, so that more recent teaching with computer courses comes only now to fruition, but still lacks the easy voice capability. More about this is discussed in Section E.

The research during the second time period at RPI in Section D is described in close to 140 publications. It was designed to create better thermal analysis and make fullest use of the new computers. Section D starts with a full description of ATHAS, the *Advanced THermal Analysis System*. Figure 12 illustrates treatment of data of newly analyzed glassy and crystalline polymers. Section D ends with a major effort to understand mesophases.

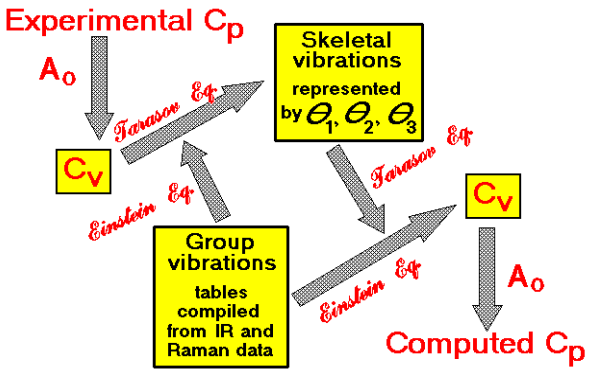

Figure 12 *The ATHAS, developed for the computation of heat capacities of crystals and glasses of macromolecules.*

The idea of ATHAS is rather simple. It is based on the knowledge gained from the early analysis of the heat capacity of polyethylene, as detailed in Sect. B. To extend the initial effort to other polymers, we created a critically reviewed data bank of experimental heat capacities [82]. All data in the literature were uniformly presented in data tables, compared to parallel measurements, and judged for precision. This data bank is since 2001 under the direction of M. Pyda and available over the internet [83]. Having just an archival data bank was, however, not our goal. The data bank was to be the base for further advances. Figure 12 illustrates the scheme followed for the analysis of the heat capacity of solids that are expected to have mainly vibrational contributions to the heat capacity. First the C_p needs to be changed to C_v. Since the thermodynamic relationship:

$$C_p = C_v + TV\alpha^2/\gamma \quad (3)$$

requires information on expansivity α and compressibility γ, quantities that are often not available for a given polymer and temperature range, we adapted the Nernst-Lindemann equation as:

$$C_p - C_v = 3RA_o C_p T/T_m^o \quad (4)$$

where A_o can either be fitted to limited experimental α and γ data, or taken as a universal constant of 3.9×10^{-3} K mol J^{-1} [84]. The next step was the computation of the heat capacity contribution of the group vibrations using information based on infrared and Raman spectra. The calculation involves mainly Einstein functions [16] and combinations of one-dimensional Debye functions [17]. Subtraction of this contribution from C_v yields the remaining skeletal heat capacity. The inversion of the skeletal heat capacity gives the parameters of the Tarasov function, Θ_3 and Θ_1 [18]. The computation programs and a discussion of the results are given in [85]. The value of Θ_3 represents approximately the upper frequency limit of the intermolecular vibrations, and Θ_1, the upper limit of the intramolecular skeletal chain vibrations. This analysis accounts for the left half of Figure 12. By computation in reverse, as indicated by the right half of the figure, C_p due to the vibrations in the solid can be calculated at any temperature. Figure 4 shows the results of such a computation.

Starting at about 250 K, an increasing deviation from the vibrational heat capacity occurs. This could later be linked by molecular dynamics simulation to defects in the crystal (see Sect. E). Analyses for more than 100 polymers are now available in the ATHAS Data Bank [83]. Starting with 1981, a biannual ATHAS Report was issued, describing the progress in thermal analysis (see Chapter 8, Figure 69 and Chapter 9, Figures 19 and 44). The eighth report of 1995 concluded this series. Further information becomes available as soon as it happens by listing on the internet, a practice that is now continued from the University of Rzeszow by Dr. Pyda.

The theoretical description of heat capacities of liquids was attempted with approximations based on statistical mechanics, but did not lead to simple analyses [86]. Liquid polymers and solid polymers with insufficient experimental data, as well as copolymers and blends are better analyzed using empirical addition schemes based on group contributions [87]. Empirically, heat capacities are predictable with an accuracy of 3–5%. Once the analysis is completed, the integral thermodynamic properties can be evaluated, as shown in Figure 5. The needed transition parameters are usually measured independently and extrapolated to equilibrium. A listing of the presently best available information is also contained in the data bank [83].

The study of glassy polymers involved di-block and tri-block copolymers of styrene and α-methyl styrene and a comparison with a blend of the same composition of components [88]. A number of noteworthy observations were made. First, in the micro phase-separated block

copolymers the glass transitions were broadened asymmetrically. In the chosen copolymer system, the upper end of the glass transition of the polystyrene phase (T_g = 373 K) is spread to higher temperature since it is surrounded by glassy poly(α-methyl styrene). At the beginning of the glass transition of poly(α-methylstyrene) (T_g = 441 K), it is surrounded by polystyrene melt, so that its T_g is shifted to lower temperature. Ultimately, both glass transitions merge and cover the full 68 K between the two homopolymer glass transitions. The blend of homopolymers of the same two components was compatible at low molar masses and incompatible at higher ones. In this case the glass transition could be used for evaluation of partial or full phase separation. The glass transition of the solution was shifted, as expected, to an intermediate temperature, but it was also symmetrically broadened. This broadening of the glass transition of polymer solutions is an observation that can be made also on polymer solutions in low molar mass solvents. Only if the two components are fully mixed, as in a random copolymer, is the glass transition as sharp as in the homopolymers [89]. The symmetric broadening is expected to result from the neighbors along the chain direction fixed by the synthesis, i.e., homopolymers in solution must remain unmixed in at least one dimension.

Poly(tetrafluoroethylene), PTFE, is a polymer that crystallizes easily, so it was difficult to observe its glass transition. A search of the literature indicated 36 different T_gs spread over 300 K. Quenching a copolymerized PTFE with a small amount of hexafluoropropylene led to a sample of only 17% crystallinity. With help of the data bank heat capacities, a broad glass transition centering at about 200 K could be identified [90]. This was one of the first times the utility of the data bank was made use of. With the limiting heat capacities of both liquid and solid well established, the glass transition can be identified, even if it spreads over more than 100 K.

The glass transitions of partially crystalline polymers are of particular interest. An analysis of poly(ethylene terephthalate) and several other polymers showed that the hysteresis observed on slow cooling followed by fast heating did not occur on all of the semicrystalline polymers. In addition, the increase in heat capacity at T_g was often reduced more than expected from the independently measured crystallinity. This means that above the glass transition temperature the heat capacity is less than expected [91]. This observation was quantified on poly(oxymethylene) and the missing melt was called the *rigid-amorphous fraction*, (RAF) [92]. The rigid-amorphous fraction has later proven to be of great importance in the understanding of mechanical properties. It gives a quantitative measure of a distinct third phase in partially crystalline polymers, and expands on the concept of the nano-phase-size *amorphous defects* [21].

After a third leave at RPI, Volume 3 of Macromolecular Physics was completed [93] see pages 8-58, 62–63). It dealt with polymer melting. Also, an extensive review of the basis of thermal analysis was prepared [94]. Besides updates of the audio courses [55], supported by a fourth leave (3rd sabbatic, 1980/81), a computer-based freshman chemistry lecture was completed, supported by a work book. This had the aim to introduce students to the applied side of chemistry and teaching engineering applications through polymer and solid state knowledge [95].

With new insight gained from scholarly work, new observations on the glass transition, and the backing of the growing data bank, many polymers were analyzed from 1975 to 1988 using the ATHAS of Figure 12. Much more information could be extracted from thermal analyses because of the ability to understand the irreversible transitions, as shown in Figure 9, the knowledge of the equilibrium limit, the quantitative information on C_p due to vibrations only, and the measured or extrapolated liquid C_p. The polymers studied covered a wide range. Inorganic polymers were a polyphosphate [1] and selenium [96] with intriguing chemical reactions that allow chains to

rearrange. Inorganic substances included also two-dimensional polymers such as graphite and the group IV chalcogenides [97]. They are described with two-dimensional Θ-temperatures. The basic, synthetic, flexible macromolecules polyethylene [98], poly(ethylene terephthalate) [99], poly(4-methyl-1-pentene) [100], poly(oxyethylene) [101], fluoropolymers [102], and polypropylene [103] were revisited to improve the data bank and to establish transition parameters. A series of more modern, stiffer-chain molecules were analyzed, including polyparaxylylene [104], poly(oxy-1,4-phenylene-oxy-1,4-phenylenecarbonyl-1,4-phenylene) (PEEK) [105], poly(oxy-2,6-dimethyl-1,4-phenylene) (PPO™) [106], poly(ethylene-2,6-naphthalene dicarboxylate) [107], poly(butylene terephthalate) (PBT) [108], poly(thio-1,4-phenylene), and poly(paraphenylene) [109].

The newest class of polymers of this time period were macromolecular liquid crystals, LCs. Macromolecular LCs were first observed in form of lyotropic[1] systems [110] and discussed in terms of segmental rigidity [111]. Thermotropic, polymeric LCs[2] need no solvent. When they were mentioned in the scientific literature [112], it became of interest to find the similarities and differences to small-molecule LCs. Naturally, our data bank was ideally suited to form the basis for a detailed thermal analysis. We started first with a number of thermal analyses and tried to understand the new properties, such as LC glass transitions, heat capacities, and ordering and disordering transitions [113]. This was followed with a review of the subject that led to the discovery that many of the macromolecules classified as LCs belonged actually into a different, new class of mesophase, the conformationally disordered phase in short, *condis crystals* [61]. This new phase was obvious when applying the general *rules for the entropies of fusion based on molecular shape and flexibility* which were discovered when researching the Volume 3 of the Macromolecular Physics [93]. The rules are listed in Figure 13 together with the system of *classifying phases and mesophases*. The condis phase is closest to the crystalline state since it has neither positional nor orientational disorder of the molecule. The conformations, however, are locally mobile and disordered. They change by jumping between the different rotational isomers. Overall, this leads to the possibility of easier diffusion along the chain direction as needed for chain extension, as

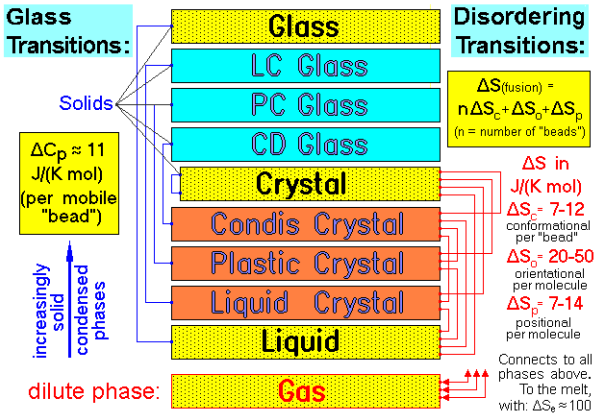

Figure 13 *The ten basic phases of matter, defined in terms of the macroscopic appearance, molecular order and mobility.*

[1] Lyotropic liquid crystalline phases derive their anisotropy from interactions with solvents.

[2] A thermotropic LC has an LC/isotropic phase transition temperature at T_i, in contrast to a lyotropic LC that usually does not lose its structure at higher temperature.

discussed in Sect. C. This discovery led me to spend my last sabbatical leave in 1986/87, with the help of a Humboldt Prize, at the Universities of Freiburg and Ulm (Germany). Many discussions and research projects were undertaken to learn the intricacies of the condis phase. The experience of this year is summarized in Reference [62] and a series of papers were published that deal with the differences between the mesophases [114]. On my return from Germany, I was offered a Distinguished Scientist position at UTK and ORNL, and chose early retirement from RPI as of Jan. 1, 1988, after almost 25 years of service and 244 publications (see pages 8-129–132).

E. MOLECULAR MOTION AND DISORDER (1988–1996)

It was mentioned in the Introduction that time goes fast. This must be true since it only seems like yesterday that we moved ATHAS from RPI to The University of Tennessee and Oak Ridge National Laboratory in 1988 (Chapter 9, pages 9-14–19). With only one student, Mr. Xenopoulos, research was begun. By 1996, this work was documented in approximately 150 papers. The new teaching effort had produced two textbooks on thermal analysis [115, 116] and a new, exciting computer course displaying text, figures, and hypertext. The computer course is available over the internet (see Chapter 8, Figure 74), the last version has been released in 2007 [117].

Thermal analysis experienced a stage of rapid development during this period of time. It was brought about by the introduction of faster and more precise calorimeters and the possibility of better data analyses. The main problem of calorimetry invariably is the difficulty to control heat losses. The measurement of heat capacity by DSC has always been troubled by the need to make a series of three runs: First, a baseline-scan with empty sample and reference pans needed to be made, to be followed by a calibration scan (usually with sapphire), and then concluded by the sample run. For critical work, this should even be followed by a repeat of the baseline scan to be assured that nothing has changed during the first three runs. As an improvement, we developed a *single-run DSC* based on a commercial triple-calorimeter (see page 9-15). After an initial calibration of the asymmetry of the three pan positions, a single run could produce good heat capacities [118].

A much more revolutionary approach was offered by temperature-modulation of the DSC (TMDSC). The sample temperature, T_s, and the temperature difference, ΔT, show in this case a small, sinusoidal variation of frequency ω [119]. Typical modulations of T_s are from 0.1 to 1.0 K at 0.1 to 0.01 Hz. Since heat losses occur most likely with a different frequency, they can easily be eliminated from the calorimeter response. Figure 14 illustrates the method of modulation and gives a comparison between DSC and TMDSC. The details of the mathematical descriptions and applications are available in the literature [120]. Of importance was the proof that a steady state can be achieved even in the presence of modulation when e^{-Kt/C_s} becomes negligible:

$$T_s(t) - T_o = q\left[t - \frac{C_s}{K}\left(1 - e^{-Kt/C_s}\right)\right] + A_{T_s}\left[\cos\varepsilon\sin\omega t - \sin\varepsilon\cos\omega t + \sin\varepsilon e^{-Kt/C_s}\right] \quad (5)$$

where $T_s(t)$ is the time-dependent, modulated sample temperature, T_o, the starting temperature, q, the underlying, constant heating rate, C_s, the heat capacity of the sample calorimeter (pan + sample), K is the thermal conductivity constant, and ε is the phase-shift relative to the block-temperature. The phase-shift ε can be expressed by Eq. (6), and the heat capacity difference ($C_s - C_r$) can be extracted

from the maximum amplitudes A of the modulation, as set for the sample temperature T_s, and measured for the temperature difference ΔT and is written as Eq. (7):

$$\sin\varepsilon = \frac{\omega}{\sqrt{\left(\frac{K}{C_s}\right)^2 + \omega^2}} \tag{6}$$

$$(C_s - C_r) = \frac{A_{\Delta T}}{A_{T_s}} \sqrt{\left(\frac{K}{\omega}\right)^2 + C_r^2} \tag{7}$$

where C_r is the heat capacity of the reference calorimeter (empty pan). Besides measurement of heat capacity, it is also possible to distinguish between thermal processes that occur equally on heating and cooling (such as C_p), and others, that do not (such as the latent heats during crystallization/melting). The temperature modulation of the DSC, thus, is an important new technique for the study of the many irreversible processes possible in polymeric and other materials [120].

The prior research period, described in Section D, closed with the discovery of the importance of conformational motion and disorder in polymers. Such increase in disorder is measured by an increase in entropy beyond that given by the vibrational heat capacity. Examples are the beginning of devitrification on heating (see Figure 3), the introduction of defects below the melting temperature (see Figure 4), and the mesophases transitions (such as liquid crystals, plastic crystals and condis crystals) as summarized in Figure 13.

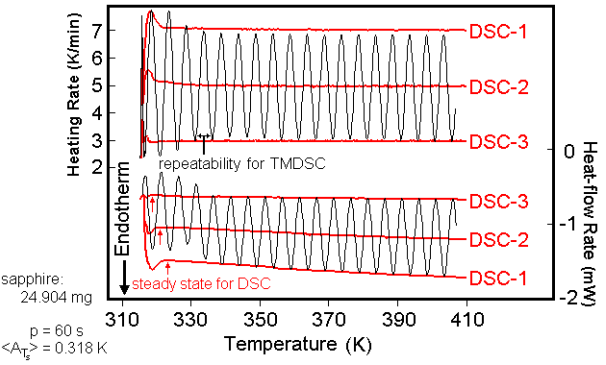

Figure 14 *A comparison of DSC and TMDSC. (For details see [120], as well as Section F, below [158]).*

A research program on molecular dynamics simulations of crystals was developed in cooperation with Dr. Noid of ORNL. His programming skills allowed to simulate motion of up to 30,000 atoms for as long as 10^{-10} s by integrating the classical equations of motion from a chosen initial state. The results are described in about 35 joint publications. Over the years, the simulations took almost 8,000 h of supercomputer time. Overviews are given in [45], and Figure 15 demonstrates the information of importance to thermal analysis. In the upper left of the figure, one can see skeletal vibrations within a crystal as snapshots of segments of seven neighboring chains. The upper right plot shows the increasing concentration of gauche bonds that can be counted in a crystal that should ideally have only rotational trans-isomers. The change of a trans-conformation to a gauche-conformation is the basic large-amplitude motion of flexible polymer backbones. The beginning of a sizeable concentration agrees with the increase in C_p seen in Figure 4. The same

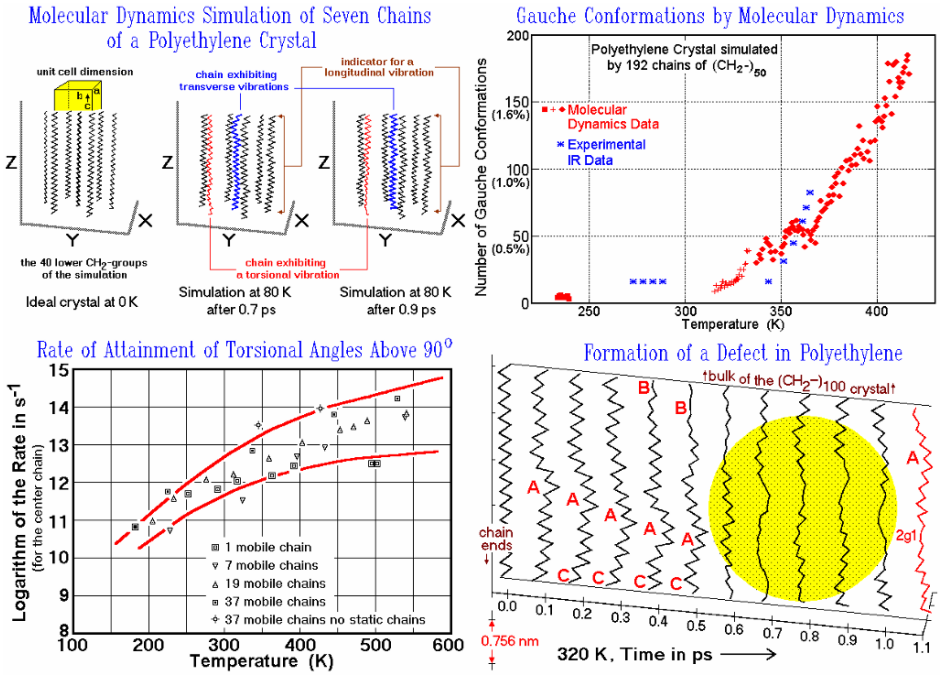

Figure 15 *Molecular dynamics simulations showing skeletal vibrations, concentration of gauche conformations, rate of formation of gauche bonds, and the mechanism of kink formation (A, B, and C indicate transverse, torsional, and longitudinal vibrations, also seen in the upper left figure).*

increase in C_p was found for all *n*-paraffins [48] and other polymers with sufficiently long paraffinic chains. The gauche-concentration is rather low, but the rate of gauche-bond formation per bond is enormous, so that each bond in the crystal changes frequently. The curves were derived for chains of $(CH_2^-)_{100}$ at different simulation conditions either enclosed in rings of static chains (constant volume simulation) or without static rings (constant, zero-pressure simulation). The corollary of low concentration and fast rate of formation is a picosecond lifetime. Combinations of two gauche defects lead to a kink, a more stable point defect in polymer crystals which was proposed earlier [121]. With the help of kinks, crystal deformation can be understood better [45, 122]. The lower right drawing in Figure 15 illustrates kink formation inside a crystal as a function of time. One can see that the collision of three skeletal vibrations provides the energy for the defect formation. Based on such simulations, it was possible to visualize for the first time the thermal motion in crystals on a molecular scale (see also Chapter 9, Figure 18B). An overall discussion of the defect solid state of polymers became thus possible, based on experiments and simulations [45].

The molecular dynamics simulations are supported by thermal analysis as a macroscopic tool. (See also Chapter 9, Figure 44.) To avoid the complications known to exist in the long macromolecules due to chain folding, we also analyzed a series of symmetric tetra-*n*-alkyl ammonium

salts. They are known to be rich in defects [74]. The calorimetry was supported by microscopic information from ^{13}C solid state NMR to get direct experimental information on the mobility of specific atoms, and by X-ray diffraction for structure analysis [123]. Combining these results with earlier work [114], it was possible to find the signature properties of plastic crystals, liquid crystals, and condis crystals [124] (see also Figure 13). Macromolecules which are located at the border between condis crystals and main-chain liquid crystals could now be identified by their phase structure, heat capacity, and large-amplitude mobility [125]. It was interesting to note that in many of the polymeric and small molecules which show mesophases, some of the disordering occurs outside of the transition region. Recognizing such gain of conformational disorder outside of the transition region infers that simple analyses using baseline separation of the heat capacity leads to substantial underestimations of the heats of transition.

For a long time we hesitated to study polymeric fibers by thermal analysis because of their complex structure. The observation that crystals in highly drawn fibers could persist far above equilibrium [126, 127] was explained by the strain transmitted from the crystals to the amorphous defects (via tie molecules in fringed micellar crystals, see Figure 11). With the discovery of the rigid-amorphous phase, RAF [91, 92], it became clear that on drawing of fibers, the RAF can change to an *oriented intermediate phase*. With two oriented and one amorphous phase, the number of possible phase-structures increases considerably, as can be derived from Figure 16. Only the phases 1, 2, and 3 can be in equilibrium. All others are metastable. Size, orientation, shape, structure, mobility, and interfaces of the phases need to be considered for the understanding of the basic structure-property-processing triangle.

We were helped by the X-ray expertise of Dr. W. Busing of ORNL (see page 9-17). He developed full-pattern Rietvelt fiber analyses of, for example, poly(ethylene terephthalate) [128]. Figure 17 shows clear structural evidence of a substantial amount of an oriented, intermediate phase. Its amount and orientation determine the fiber modulus and tenacity as is shown in Figure 41 of Chapter 9. The crystallinity and the perfection of crystals are of secondary importance [128]. Another fiber similarly analyzed is gel-spun, ultra-high molar mass polyethylene [129]. In this case almost all chains are parallel to the fiber direction, but not all participate in the crystal. By solid state ^{13}C NMR we could show that the not-crystallized chains had a much higher mobility than the crystals and only a very small amount of fully amorphous material was present. These structure, order, and mobility results are included in Figures 44D & E of Chapter 9 and are described on page 9-48.

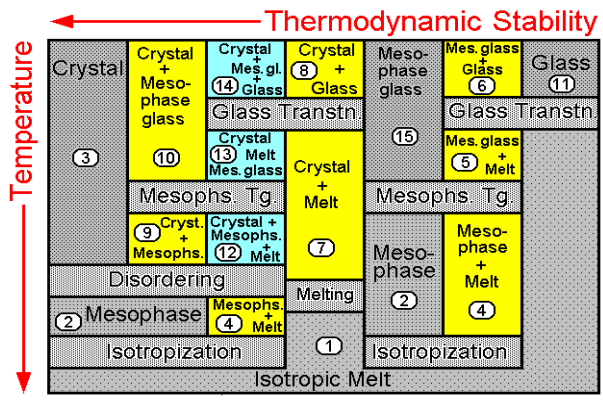

Figure 16 *Phase diagram of a three-phase system with metastable states. The equilibrium states are found on the left side, transitions are indicated by the densely dotted boxes, the numbers indicate the 15 possible phase areas.*

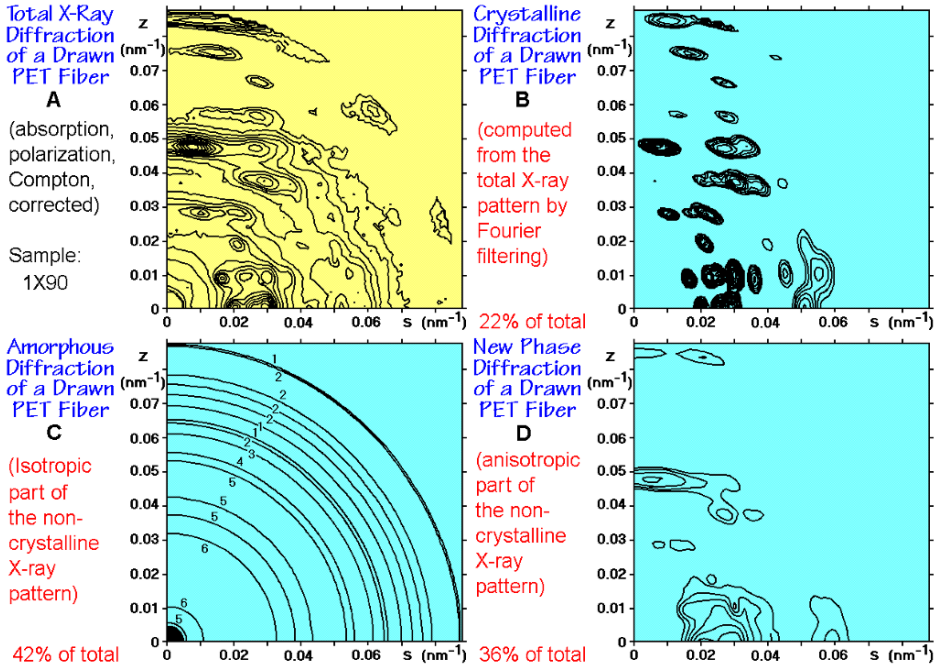

Figure 17A–D *Rietvelt analysis of poly(ethylene terephthalate) fibers. The X-ray diffraction pattern of* **A** *arises from the superposition of the three components* **B–D**. *(Three-phase structure).*

The completion and computerization of the ATHAS Data Bank accelerated at UTK and ORNL with the possibility to employ more permanent coworkers [82] (see pages 9-14–17). Thermal analysis of aliphatic polyamides (nylons) [130] indicated a major increase in mobility and disorder of methylene sequences in the crystals before melting [131]. Quasi-elastic neutron scattering confirmed an almost liquid-like conformational mobility within the crystal [132]. A new direction grew out of the research about the polyamides when it was observed that the known heat capacities of a few poly(amino acids) (nylon 2) did not fit into the series of homologs [130]. The problem was resolved by re-measuring not only the few available data, but establishing information for all homo-poly(amino acid)s and some copoly(amino acid)s that can be made out of the 20 naturally occurring amino acids [133]. It turned out that at room temperature and above, all prior measurements had up to 50% errors due to slow evaporation of water. As soon as this groundwork with poly(amino acid)s was laid, we turned to solid proteins. The first step was to see if the ATHAS method shown in Figure 12 is also applicable to biological materials. The proof is in the Figure 18. The root-mean-square errors of the heat capacity due to skeletal vibrations of a protein are shown to possess a minimum for unique values of Θ_1 and Θ_3 of the Tarasov equation [134]. This observation opened the doors for thermal analyses of proteins and allowed a discussion of their stability (G), disorder (S), and enthalpy (H), as was shown for polyethylene in Figure 5.

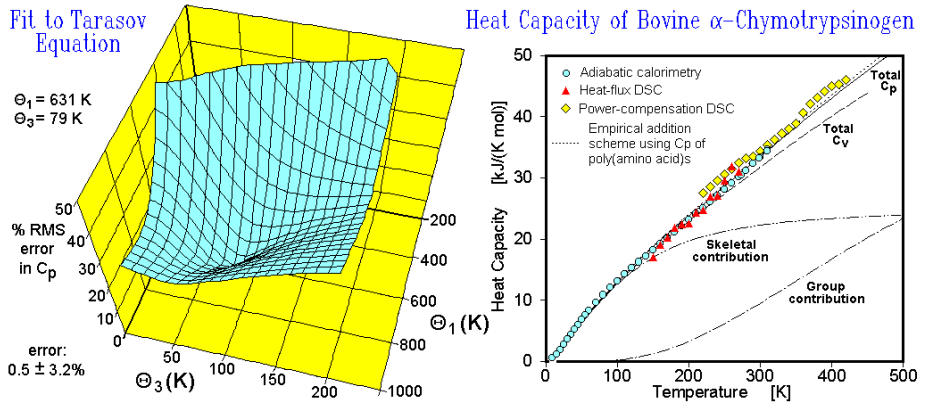

Figure 18 *Minimization of the error for the description of the skeletal heat capacity of the solid protein bovine α-chymotrypsinogen of type II with 245 amino acid repeating units and an overall molar mass of 25,646 Da. The molecule has a total of 3005 skeletal vibrations [134]. The right graph is a comparison of the calculation and measurement of the heat capacity.*

A series of topics that was of greater importance for the future closes this Section E. To get to at the root of the problems of thermal analysis, all aspects of phase structure, morphology, and molecular motion must be combined with the macroscopic thermodynamics. For crystals of polymers, this meant to start with an equilibrium single crystal as the base for judging defect structures. For polyethylene [135] and some crystals grown during polymerization [21, Vol. 2] it was possible to produce crystals sufficiently close to equilibrium for direct analysis. Even more challenging was the effort to make *single-molecule single-crystals* [136]. The crystals made proved still metastable and could not be annealed to equilibrium (see Figure 43 in Chapter 9). It may also be of value to see the changes when going to two or three molecules per crystal and to study how molecular domains can fit within the confines of the crystal morphology. Direct observations of atoms is now possible by the method of atomic force microscopy (AFM). We bought an early AFM and could, indeed, 'see' a large amount of atomic and molecular detail [137] (see Chapter 9, Figure 42 and pages 44–45). There is hope that this tool for nanotechnology may permit to check mechanical properties, and why not perform thermal analysis on a nanometer scale? This effort had made progress in the following 10 years and will be discussed in Sections F and G.

New materials are constantly being produced. A very exciting group of compounds were the fullerenes. Shortly after these became available, we analyzed C_{60} [138] and C_{70} [139] and compared them to the two-dimensional graphite. As one would expect, plastic crystal phases with beginning motion outside the transition region could be quantified by the ATHAS analysis. At room temperature these highly symmetric fullerenes rotate in the crystalline state which remains stable to very high temperatures. The large spaces in the crystal between the molecules can hold small molecules like toluene with almost chemical-bond-like stability and hinder their mobility. Again, thermal analysis and solid state NMR were the tools that could resolve this behavior by quantitative interpretation of the transitions and increases in heat capacity outside the transitions.

Thermal analysis has progressed substantially in linking microscopic causes to the observed macroscopic observations. Whenever such a link is well understood, predictions of the properties of new materials can be made. Sometimes, these predictions are good enough to almost obviate the need for further experimentation. This leaves, however, the areas that are not supported by a well-worked-out theory. By now, it may then be possible to predict with neural net calculations. The first attempts at such estimations in the field of thermal analysis showed promise [140].

F. REVERSIBLE MELTING AND THE RIGID-AMORPHOUS PHASE (1996–2001)

The discussion of research about thermal analysis and related fields at UTK and ORNL until my retirement in 2001 is divided between the previous Section which covered the time until my 65th birthday (see the pages 9-51–54) [141], and the present Section F. Together, the two periods represent the most productive time of my professional carrier, they account for approximately 250 publications. The close cooperation with senior members of the Polymer Group of ORNL added experimental breadth and expertise to the effort to understand polymers and permitted combined supervision and teaching of postdoctoral associates and students (see pages 9-14–17 and 50). Figure 40 in Chapter 9 is a picture of the combined researchers in 1990. Sections G and H, then, cover the time after retirement, separated by the closing of the ATHAS Laboratory in 2006.

The central theme of our study was always the probing of the amorphous, crystalline, and mesophase structures of different molecular mobility on the macroscopic (thermodynamic) and microscopic (atomic) level. The schematics in Figures 10, 11, 13, and 16 summarize the basis for thermodynamics as it developed over the years. In Section E much was added to the picture of solid polymers reached in the 1970s [21, 93]. The next level was reached by 1996. It was broadly discussed in St. Petersburg, Russia, at the 2nd International Symposium on 'Molecular Order and Mobility in Polymer Systems' [142]. Two specific reviews tie the progress described in Section F to the prior literature. The first gave an initial definition of *macro*, *micro*, *and nano phases* for small and large molecules [143]. The second dealt with results derived from quantitative TMDSC [144]. Based on the 350 literature citations in these two reviews as they arose from a large number of laboratories, it was concluded that the ordering of flexible macromolecules results commonly in *globally metastable*, *semicrystalline polymers* of micro and nano phase agglomerates of crystalline and rigid and mobile amorphous or partially oriented phases. The crystals, additionally, may contain local subsystems which *melt reversibly* [116, 145]. In 2000, progress of this research was extrapolated into the 21st century [146]. By now, in 2010, one can note already prior unforeseeable results from modern, super-fast scanning and microcalorimetry of isolated nano phases.

Section F is divided into six topics. (**a**) The new instrumentation of TMDSC and the mastery of temperature modulation—its ability of data-deconvolution increases the precision of heat capacity evaluation. (**b, c**) The separation of equilibrium heat capacities from latent-heat effects—it permits to better understand glass and order-disorder transitions. (**d**) The intermediate rigid-amorphous phase as an integral part of the description of semicrystalline polymers—it is, as a third phase, often a nano phase, and may also become partially oriented on deformation. (**e**) The expansion of the data bank—it supports the concept of *decoupled chain segments in nano phases* by the analysis of newly available synthetic and biological macromolecules. (**f**) Information from *single-molecule single-crystals*, and the use of microcalorimetry on very small samples—it leads to direct calorimetry on the basic metastable systems (see also Figures 42 and 43 in Chapter 9).

(**a**) Instrumentation of TMDSC matured during this second research period at UTK and ORNL, 5–10 years after the first use of temperature modulation [119]. A first problem was the asymmetry of the twin calorimeters. In standard DSCs asymmetry is corrected by measuring the heat-flow rates of a run with two identical, empty pans. It is more difficult to correct TMDSC. On Fourier transformation into the frequency domain, the phase-shift of the reversing heat-flow rate in the time domain loses directiveness, needed to correct (±) the amplitude of the reversing heat-flow rate [147]. A preliminary solution was to create a known asymmetry by using pans of different mass. By now, calorimeters with asymmetry correction are available based on modeling using an electrical-analog circuit (Q 1000 MDSC of TA Instrument Inc., Tzero software®) [148].

A similar computation was fitted in our laboratory to the Mettler-Toledo DSC, as shown in Figure 19 [149]. The strong frequency dependence of the heat capacity below periods of about 100 s for typical commercial instrumentation can be corrected for, as seen from the center curve. Turning to a third DSC in Figure 20, it is shown for sawtooth modulation of the sample temperature, that multiple frequencies can be analyzed simultaneously by Fourier transform of the resulting heat-flow-rate response [150]. The Fourier components are seen in the upper left curves. Using the five harmonics indicated, and four different sawtooth periods, the 20 data points could be generated. Analyzing the data by applying Eq. (7) with an empirical function τ instead of C_r/K, yields a frequency dependence of the heat capacity as shown in the lower left graphs. At low frequencies, the heat capacity changes linearly with the square of frequency, as is expected from Eq. (7) and seen in the bottom left insert. The reversing heat capacity is then simply:

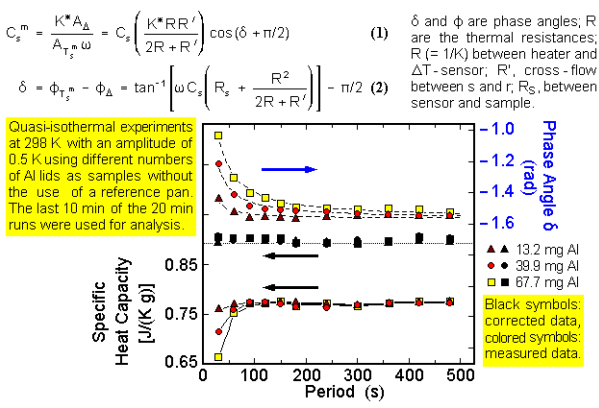

Figure 19 *Measurement with a Mettler-Toledo TMDSC of type 821 as a function of frequency $\omega (= 2\pi\,\text{period}^{-1})$. The measured heat capacity is C_s^m, A indicates the amplitudes of sample temperature, T_s, and the temperature-difference response is Δ. The value of C_s is the (known) heat capacity of Al, and K* is the calibration constant which fits the vertical offset of the heat capacity, found by analogous measurements with sapphire.*

$$mc_p = \frac{A_{HF}}{A_{T_s}\omega}\sqrt{1 + [\tau(m)]^2\omega^2} \qquad (8)$$

with τ (for a given sample) still being mass dependent. As one exceeds $\omega^2 = 0.5$ (a period of about 10 s), strong deviations start, but τ remains a continuous function of frequency. Since different samples have different values of τ, the sapphire and sample run must be calibrated separately. By additionally investigating the linear heating and cooling segments of the sawtooth modulation, one can obtain standard DSC data for a comparison to the Fourier-transforms of the various harmonics

[151]. In this case, direct information about an irreversible process can be obtained, which otherwise is available only indirectly from the difference between total and reversing responses.

A more complex sawtooth with close-to equal amplitudes of the different harmonics was created by us by the linking 14 linear heating and cooling segments [152]. This complex sawtooth can be generated in any standard DSC which permits to link and repeat the different segments. With these methods, measurements of C_p which approach ±0.1% precision were possible, approaching the precision of the classical adiabatic calorimetry [153].

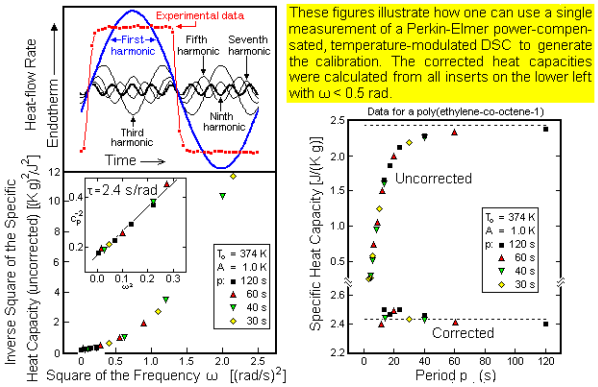

Figure 20 *Measurement with a Perkin-Elmer TMDSC of type 7 as a function of frequency* $\omega (= 2\pi\,\text{period}^{-1})$. *The specific heat capacity can be corrected with Eq. (8) using a constant* τ *which above a period of about 10 s changes only with sample type and mass. Below 10 s it becomes also frequency dependent. The value of* τ *is the slope of the curve in the lower left diagram.*

The data for high-precision heat capacity determinations were generated with quasi-isothermal measurements which consist of a modulation about a constant base temperature for 20 min or longer. The first few modulation cycles were discarded, to avoid the initial approach to a steady state, seen in Figure 14. This method is of particular importance for samples which change their phase structure during the measurement and absorb or generate irreversible latent heats. The quasi-isothermal measurement, then, can be extended until the irreversible processes cease. In the absence of slow irreversible changes, TMDSC with an underlying heating rate is also capable to produce improved heat capacity data [154]. In the presence of slow irreversible processes, such TMDSC yields an apparent heat capacity which must be separated from the time-dependent contributions.

The temperature gradients within the calorimeter were studied by direct, contactless, infrared thermography [155]. Fast, multiple-frequency modulation could be achieved with the infrared light by applying a program of pulse-width changes. In these infrared modulation experiments, the calorimetric response was detected by standard DSC [156].

Detailed modeling of TMDSC [157] allowed to collect enough experience to tackle data interpretation when large amounts of latent heat are present which destroy linearity and stationarity of the measurement, as well as to discuss the usefulness of the introduction of a complex heat capacity [158, 159]. Figure 21 is an example of simulation of reversing heat-flow rates, $HF(t)$, on instantaneous melting, reversed by instantaneous crystallization in the next cycle. As indicated, the total heat-flow rate $\langle A_{HF} \rangle$ and its smoothed value are largely different from the standard DSC result. This is caused by the loss of stationarity of the sliding average $\langle A_{HF} \rangle$ which must be changing close to linearly to allow a proper deconvolution of $HF(t)$ from the total heat-flow rate [160].

(**b**) The first detailed study of time-dependent heat capacity was concerned with the glass transitions of amorphous polystyrene and of poly(ethylene terephthalate) of different degrees of

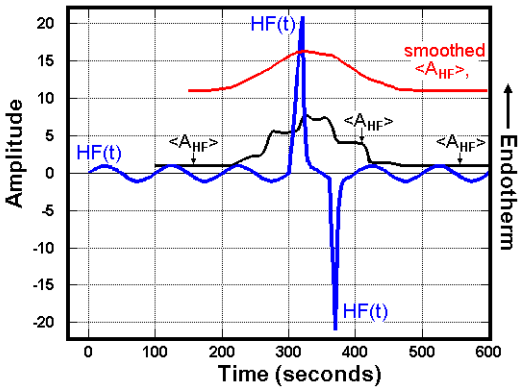

Figure 21 *Simulation of a single, equilibrium melting followed by crystallization in TMDSC. The heat-flow rate, HF(t), when averaged over one sliding period of modulation is <A_{HF}>. It is not equal to the total heat-flow rate obtained by standard DSC because of the missing stationarity on deconvolution. The smoothed <A_{HF}> is the usual result given by TMDSC.*

crystallinity [161]. Figure 22, on page B-27, illustrates the approximate separation of the non-reversing and reversing heat capacities of polystyrene on TMDSC, and the extrapolation of the experimental data to a wider range of frequencies. Note that the non-reversing heat capacity represents the difference between the total heat capacity, measured as the sliding average over one full modulation period, C_p(total) = <mc_p>, and the reversing part, mc_p as derived from Eq. (8), which is calculated from the first harmonic of the response of the TMDSC to the modulation of the sample temperature. This procedure approximately separates the heat capacity from the hysteresis effect due to the thermal history of the sample. This hysteresis effect is shown in the lower left of Figure 22. From the experiments at different modulation periods, a relaxation time can be assessed, and the heat capacity can be extrapolated to higher frequencies. The results are illustrated at the bottom right of Figure 22. The frequency range shown stretches from 0.01 Hz (close to the experimental data in the upper left), to 100 Hz, far from the response time of the calorimeter (period of 10 ms).

The data for poly(ethylene terephthalate), PET, where similarly analyzed. Figure 23, on page B-28, illustrates the pertinent analyses when assuming that, at least for a small temperature interval, the simple hole theory by Hirai and Eyring [36] can describe the glass transition [162]. This analysis was applied already earlier to the glass transition of polystyrene by using a first-order kinetics for the change in concentration of holes [35]. The holes are of a diameter of close to 1.0 nm and assumed to be the cause of the observed kinetic phenomena governing viscosity and the change in C_p at the glass transition temperature (seen in Figure 23, top right). The top left part of Figure 23 illustrates the response of this model to a quasi-isothermal modulation of the sample temperature. The response is only approximately sinusoidal in its change in hole concentration, N. There are two additional, small reversible contributions, one (a) being constant and one (b) is of double the modulation frequency. The major, sinusoidal contribution of frequency ω is (c). The first harmonic evaluated from the experiment can be compared only to this contribution (c) and the true reversing (non-sinusoidal) contribution given by the red curve must be computed from the boxed equation. As long as this is not done, the calculated, non-reversing contribution is in error. A further discrepancy is revealed in the lower left curves for TMDSC with an underlying cooling rate. All experimental data show a Doppler-like effect, the frequency of the reversing signal is changing with temperature in response to the changing kinetics in the glass transition region. As a result, from this frequency shift, higher harmonics appear in the Fourier analysis. The deconvoluted parts of the heat capacity show the expected modulation. This effect is not clearly revealed in the recorded data

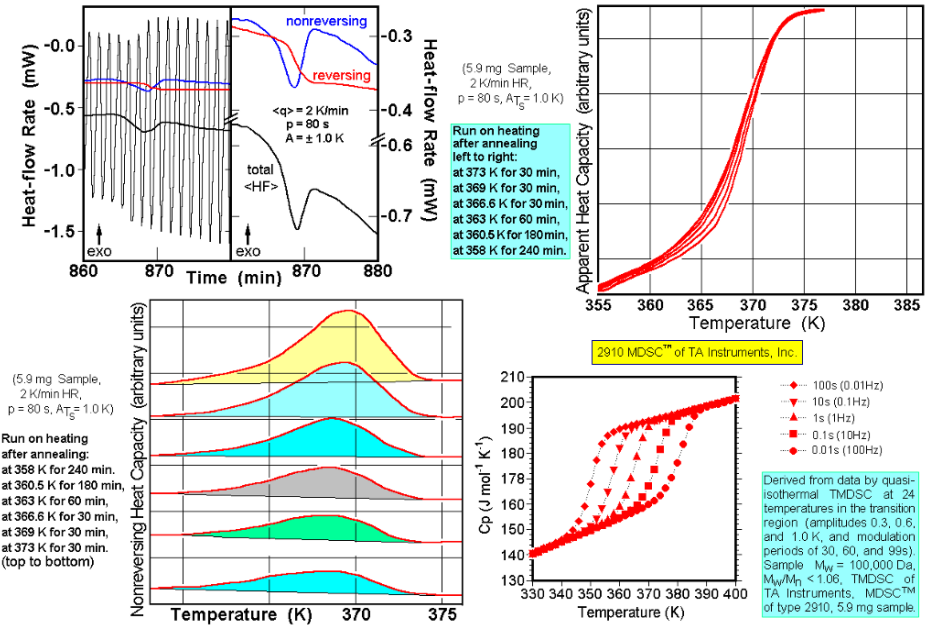

Figure 22 *Temperature-modulated DSC of polystyrene. Upper left: Raw data of the heat-flow rate, and the total, reversing, and nonreversing heat-flow rates plotted with two different scales. Upper right: Reversing C_p, showing differences for the different thermal histories. Lower left: Nonreversing C_p, illustrating the hysteresis. Lower right: Frequency-dependent, reversing C_p.*

because of the additional smoothing of the data (as indicated in Figure 21). Finally, the bottom right curves of Figure 23 illustrate that data from quasi-isothermal and TMDSC with underlying heating and cooling rates do not agree, except for the limit of very small rates $\langle q \rangle$. Trying to match the discrepancy with the hole-theory calculations is only successful in the high-temperature portion where the system is close to equilibrium. This indicates, as suggested in the earlier analyses by DDTA [34], that a cooperative model has to be developed to properly model the glass transition. Efforts in this direction have not been successful to date, an estimate of the error, however, can be made, by looking at Figures 22 and 23 (upper and lower right, respectively).

Further, quasi-isothermal analyses were used to broaden the investigation to semicrystalline samples of PET with different degrees of crystallinity, annealing, and orientation. Its glass transition region is sufficiently lower in temperature than melting, so that there is no overlap between the two transition regions. Figure 24 shows the TMDSC results. The selected curves on the left can also be used to evaluate the time dependence for the amorphous PET, to compare to Figure 23. The right plot shows the mathematical representation of the considerable broadening of the glass transition caused by crystallization and ordering, as well as the narrowing of the glass transition on annealing. The final observation is a much larger decrease in the change of heat capacity at the glass transition with crystallization than would be expected from the crystallinity, the signature of the presence of a rigid-amorphous fraction, RAF [91, 92] (for a description, see page B-15).

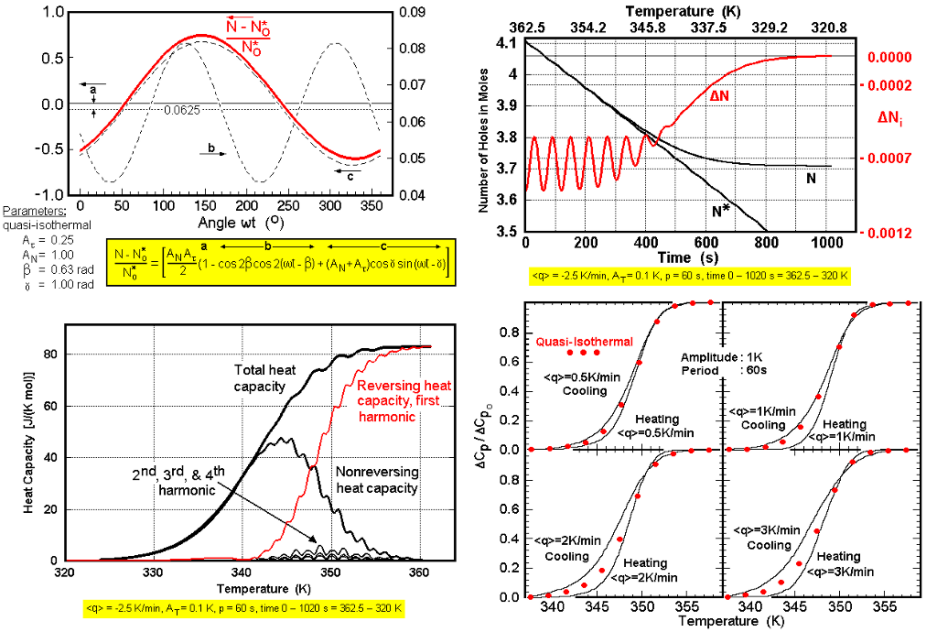

Figure 23 *Computations from TMDSC of PET using a hole theory. Upper left: The three different, normalized contributions to the instantaneous number of holes, N. (N* is the equilibrium, β and γ are phase angles, A denotes constants). Upper right: Changes in N on cooling. Lower left: C_p on cooling. Lower right: Differences between cooling, heating, and quasi-isothermal experiments.*

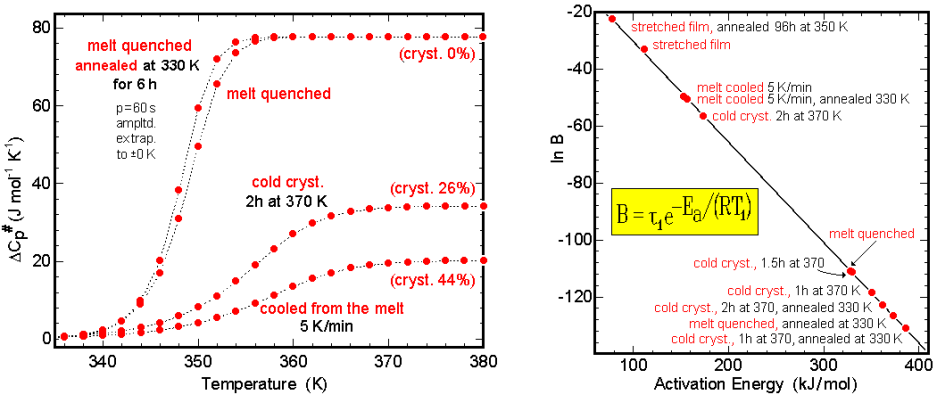

Figure 24 *Apparent reversing heat capacities of poly(ethylene terepthalate) samples of different degrees of crystallinity as measured by quasi-isothermal TMDSC (left), and the correlation of the activation energies and pre-exponential factors (τ_1 = 132.5 s, T_1 = 341 K).*

This comprehensive study of the glass transition [161] makes a connection to the prior analyzed effects of interface, pressure, and mixing effects on homopolymers, polymer solutions, copolymers, and block copolymers [35, 37, 75, 76, 88–90]. The correlation of samples on the right of Figure 24 shows the remarkable decrease in activation energy with crystallization and ordering, which, however, is compensated by a decrease in pre-exponential factors since the glass transitions of all samples begin at the same temperature, as seen in the left curves. In the case of PET and many other polymers of more rigid molecules, the RAF goes through a separate glass transition at higher temperature, as will be described below. Observations like this suggest that in such cases the RAF is a separate nano phase, while the broadening of the glass transition of the *mobile-amorphous phase* is caused by a stress transfer across the interface by incomplete decoupling of the molecules or by freezing-in of local order.

(**c**) New observations about melting of macromolecules resulted from TMDSC, the tool to probe for reversibility [144]. Quantitative TMDSC was possible after learning how to overcome the experimental problems described with Figures 19–21. First, it was necessary to identify the limits of reversible melting as seen in small molecules like indium [163] and paraffins [164]. Figure 25 summarizes these results. The TMDSC with an underlying heating rate shows that In starts melting as soon as the melting temperature is reached during modulation at point 1 in the upper left figure.

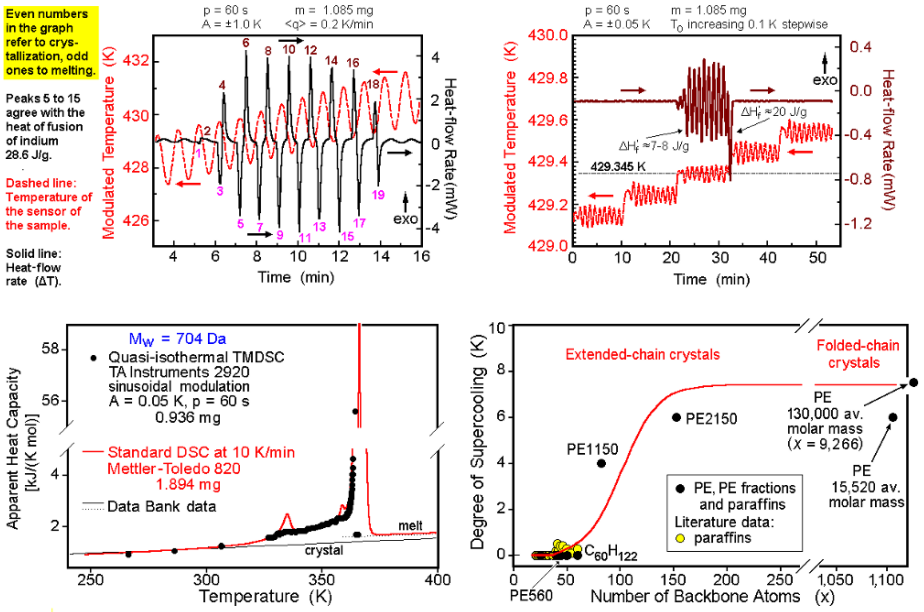

Figure 25 *Reversible melting, analyzed by TMDSC. Top left: Melting of In with an underlying heating rate. Top right: Quasi-isothermal TMDSC of In. Bottom left: Reversible melting of pentacontane ($C_{50}H_{102}$), comparison of DSC and TMDSC. Bottom right: Limits of reversible melting of paraffins and polyethylenes (PE).*

The time at or above the melting temperature, however, is not sufficient before the modulation reduces the temperature below the melting temperature and the melted portions of the crystals regrow (exothermic peak 2). This repeats itself until practically all In melts at peak 9 and a small time gap appears before renewed crystallization (peak 10). With the crystallization of peak 16 there is not enough time for crystallization, and after the melting of peak 19 the temperature does not decrease sufficiently for crystallization. The slopes between successive peaks 1–2, 3–4, 16–17 and 18–19, in connection with temperature profiles measured at the pan by IR thermometry [155], can be used to discuss the calorimeter lags. Before complete melting, the core of the sample remains crystalline, while after complete melting, it stays liquid, both with fluctuating boundaries. By reducing modulation and underlying heating rate, the reversibility of the melting can be bracketed within a few hundreds of a kelvin, as shown in the quasi-isothermal experiments (upper right of Figure 25). About 30% melts at 429.345±0.05 K, while none melts higher or crystallizes lower.

Applying this experience with indium to paraffins proves reversible melting of $C_{50}H_{102}$ with the data in the lower left of Figure 25. The standard DSC peak beyond the melting peak in the quasi-isothermal TMDSC is caused by instrument lag. As long as the heat-flow rate causing the lag is negligible, DSC and TMDSC yield identical, apparent, reversible heat capacities. Similarly, reversible first-order transition peaks could be documented for small and large liquid-crystal molecules [165]. An obvious question arose: What length paraffins can melt reversibly? This is answered by the bottom right graph of Figure 25 [166]. At much smaller numbers of backbone atoms than required for chain-folding, irreversibility is introduced by the need of *molecular nucleation* (to be considered in addition to crystal nucleation). Molecular nucleation was already suggested based on crystal growth rates (Figure 8) and rejection of lower molar mass species from a crystal of larger molar mass below its equilibrium melting temperature and even below the zero-entropy-production melting temperature of the correspondingly folded-chain crystal [21, 53, 67].

Irreversible melting was documented by TMDSC for polyethylene, poly(oxyethylenes) (POE), poly(oxytetramethylene) [166, 167], extended-chain crystals of polyethylene (PE) [168], and the crystals of Poly(oxy-2,6-dimethyl-1,4-phenylene) (PPO) [169]. In 1997, however, some locally reversible melting was discovered in semicrystalline, chain-folded flexible macromolecules like PET [170] and POE [167], despite of their globally metastable, multi-phase structure with subsystems of micro and nanometer size, mentioned above. Figure 26 illustrates three examples of close to irreversible melting and one with additional reversible melting. Details about the C_p of POE which indicate a *glass transition of the crystals* will be discussed below. The extended-chain sample of PE still has some reversing melting left, due to its broad molar-mass distribution, which however, could be accounted for quantitatively [168]. The PPO also will be further discussed below. The reversing melting of PET is typical as for many other polymers and reviewed in [144]. Other chain-folded crystals which were analyzed in our laboratory relative to their partial reversibility were polyethylene [164, 171] and some of its copolymers [172, 173], poly(trimethylene terephthalate) (PTT) [174], poly(butylene terephthalate) (PBT) [175], and polypropylene (PP) [176].

Based on these experiments and a survey of the literature [144], the locally reversing melting was modeled and the result is illustrated in Figure 27 [177]. This model emphasizes that the reversible melting is located on the growth faces of the crystals. An earlier observed reversible change of the lamellar thickness [178] is a different process. Its exothermic and endothermic heat effects have never be determined, and it does not show similar melting temperatures of reversible and irreversible melting temperatures that have been documented for polyethylene, while many more

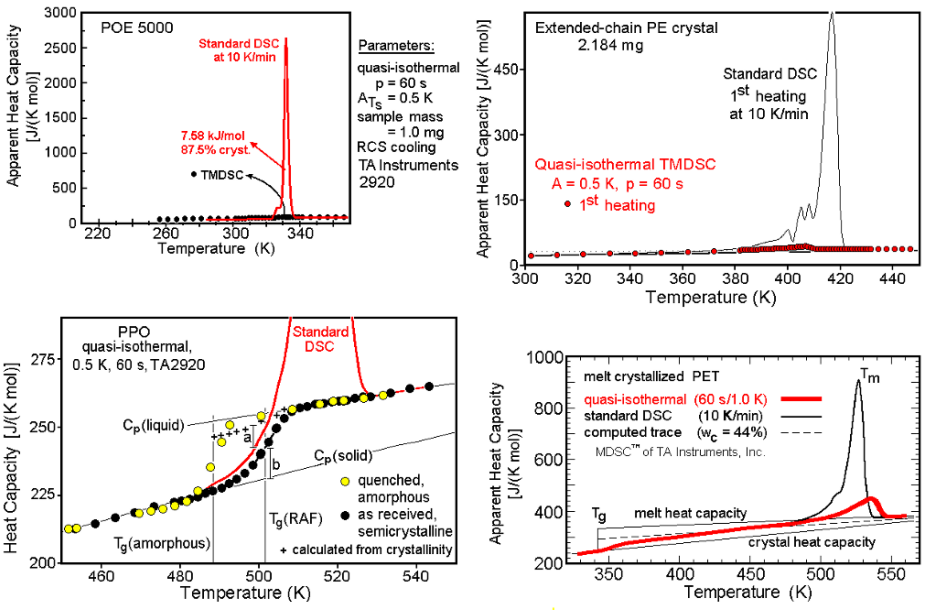

Figure 26 *The melting of polymers studied by TMDSC. Top left: Irreversible melting of extended-chain crystals of POE of a molar mass 5,000 Da. Top right: Irreversible melting of extended-chain PE. Bottom left: Irreversible melting and the glass transition of PPO. Bottom right: The first observation of partial reversible melting seen for chain-folded, semicrystalline PET [170].*

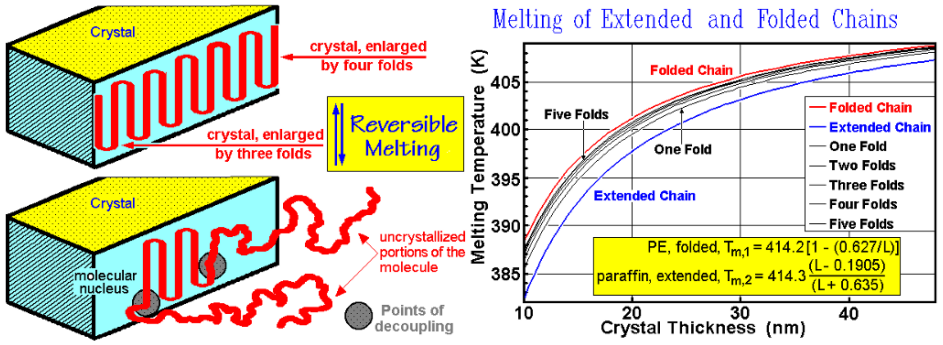

Figure 27 *Locally reversible melting on polymer crystals. On the left a schematic of a hypothetical reversible melting is drawn. The points of decoupling create subsystems on the surface with a lower, reversible melting temperature. The graph on the right documents PE melting temperatures.*

polymers show locally reversible melting on the growth face, as were proven for PP, for example [176]. (By comparison with molecular mechanics simulations [45] and the reversible behavior of other polymers [144], the different reversible change in thickness was linked to the defect creation as seen in Figure 15, followed by diffusion to the interfaces.) The important aspects of the model of Figure 27 are the *points of decoupling* which will be shown in Section G to be of rather wide importance for the understanding of polymer thermodynamics. For polyethylene, the melting point of decoupled segments can be estimated from the known T_m of folded and extended-chain crystals. The bottom equations on the right of Figure 27 permits the computation of the melting temperature, $T_{m,2}$, of the extended-chain length of a decoupled segment. The shown curves were calculated by inserting $T_{m,2}$ into the upper equation (instead of 414.2 K, the melting temperature of infinite length) and correcting the melting point lowering (in brackets) for the fraction of the surface covered with chain folds for the given segment length. (For one fold, the correction factor for the term in brackets is 0.50, for two folds, 0.67, for three, 0.75, for four, 0.80, and for five, 0.83.)

An initial attempt to extract kinetic information about irreversible crystallization and melting from TMDSC was made by Toda [179] and was also attempted during this time period in our laboratory with the polyester-imid poly(4,4'-phthaloimidobenzoyldodecamethyleneoxycarbonyl) [180]. The method was found to be applicable, but the extracted kinetics seems to be of limited use in arriving at a detailed molecular model.

(**d**) Knowing the basic information about first order transitions (as defined by Ehrenfest [181]) and the glass transition (as described by Hirai and Eyring [36]), one can tackle the temperature region between the glass and melting transitions. A frequent overlap of processes complicates the evaluation of phase structure and properties at these temperatures. In order to keep within the system of definitions for molecules (Figure 10) and phases (Figure 13), there was a need to define *nano phases*. It is insufficient to consider nano phases as small micro phases with a size approaching atomic dimensions where the phase concept becomes invalid. Micro phases have been recognized for over 100 years as having different overall properties than bulk phases (macro phases) caused by their large surface enveloping the bulk phase (see Eq. 2). To have an operational definition [182] for a nano phase, we specified in 1999 that a nano phase should be sufficiently small that it contains no bulk phase [143] (see also [183]). In a nano phase must postulate that the interior material changes its properties continually from that of the surface toward that of the bulk. Ultimately it must meet similarly altered material from the opposite surface without having reached the bulk properties. Typically this happens at distances of 1–5 nm, different for different materials.

A glass transition temperature, T_g, in a semicrystalline material which is broadened toward higher temperature does not account for a new phase. One links this effect to strain transmitted from the crystal. The strained layer at the crystal interface could be identified for PE by special electron microscopy [184]. The heat capacity for gel-spun, ultra-high-molar-mass polyethylene is shown in Figure 28 [185]. The C_p is measured by short-step DSC on heating and compared to subsequent cooling scans to check for reversibility. The upper curves show the comparison to vibrational C_p and the experimental 100%-crystalline PE as given in Figure 4. The fibers A and B are different in degree of annealing. Different levels of crystallinity and different beginnings of reversible melting of the two fibers are easily seen. The actual measured points minus the crystalline heat capacities are shown in the lower graph. They indicate broadened glass transitions, reaching much higher than shown in Figure 3. In addition, the excess in the sum of amorphous and crystalline phases beyond 100% suggests that the noncrystalline phase is partially ordered, identified as a mobile, oriented,

non-crystalline fraction by X-ray diffraction and solid state NMR [129]. (See also Chapter 9, Figure 44.). The orientation must then contribute to the heat of fusion.

A RAF, rigid-amorphous fraction, which does not participate in the glass transition of the bulk phase is seen in Figure 24 for PET. It must be a separate phase without unchanged bulk-phase in its interior. With the definition just given, it is likely to be a nano phase. Another example of a polymer with a nano phase RAF is poly(butylene terephthalate), PBT. Its TMDSC and DSC traces are illustrated in Figure 29 [175]. For the better-crystallized sample on the left, the crystallinity, w_c, of the sample can be calculated from the heat of fusion, obtained by back-integration from above the melting temperature of the apparent heat capacity, subtracting the proper heat capacity base line (red). All quantities in the equation of the heat capacity written within the figure, as well as the heat of fusion, must be considered as functions of temperature [4, 26]. This calculation cannot be continued below about 400 K since at lower temperature one can see the separate glass transition of the RAF, with a mid-temperature of about 375 K. The RAF can be evaluated at the upper limit of the broadened T_g of the mobile amorphous fraction, with a mid-temperature of 314 K. Since the lower glass transition corresponds to 42.4% amorphous phase, the difference to the crystallinity yields a RAF of 21.3%.

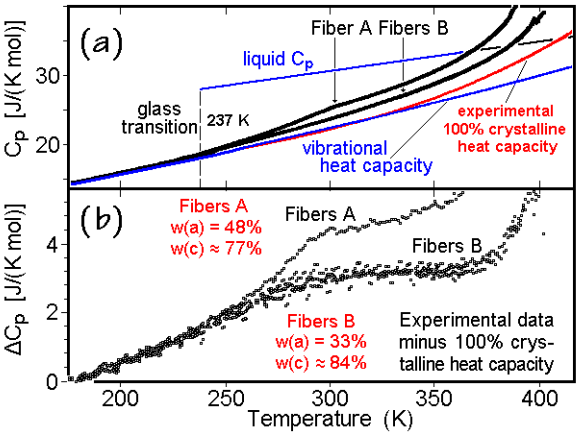

Figure 28 *Heat capacity of gel-spun polyethylene of ultra-high molar mass, compared to the heat capacity derived in Figure 4.*

The PBT sample on the right was quenched from the melt. In this case there is an overlap of cold crystallization, reorganization, glass transition of the RAF, and early melting. The standard

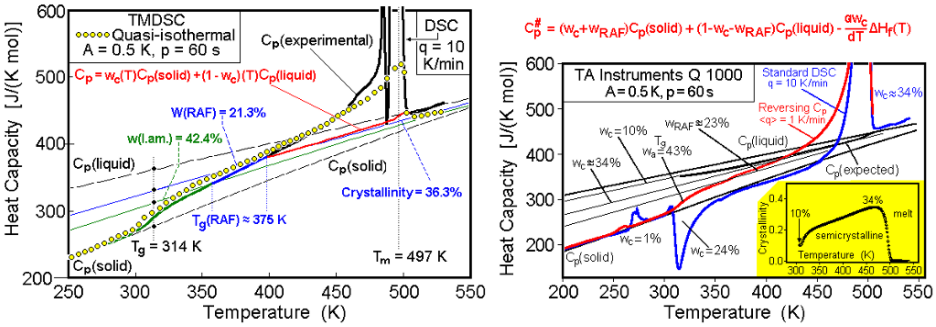

Figure 29 *Standard. DSC and TMDSC of poly(butylene terephthalate) cystallized by cooling from the melt to 36% crystallinity, shown on the left, and by quenching from the melt to 10% crystallinity, with a 24% cold crystallization (on the right). The insert illustrates the change in crystallininty.*

DSC trace (in blue) is dominated by the cold crystallization and does not allow any further analysis. From the TMDSC trace, taken with an underlying heating rate, the low-temperature glass transition is obvious, while the glass transition of the RAF is still obliterated by the reversing, broad, melting transition. Complete DSC curves can be approximated with the equation for the apparent heat capacity on top of the figure. Information about the changes of the RAF in its glass transition from the sample on the left must be inserted and the change of C_p(liquid) when becoming a glass at the low-temperature glass transition needs to be considered. The crystallinity after quenching could then be calculated to be 10%. The origin of the small endotherm below the glass transition which is frequently seen in quenched samples [108, 175] may be an instrument effect [186].

Clear evidence that below its glass transition, the RAF freezes along with the isothermal crystallization was brought in the laboratory of Prof. Schick with TMDSC by simultaneous evaluation of the reversible heat capacity and the total heat-flow rate of poly(hydroxy butyrate) for over 55 hours [187]. This experiment places the RAF directly adjacent to the crystal and the remaining mobile-amorphous phase with a lower glass transition into a separate phase at a different location within the overall metastable structure of the semicrystalline polymer.

Returning to PPO [169] in the lower left graph of Figure 26, it was noted by standard DSC for 30% crystalline samples that there was no T_g of a mobile-amorphous fraction below melting [108]. The quasi-isothermal TMDSC results prove that the glass transition of the 70% RAF occurs along with the melting. In fact, by annealing below the melting peak, the crystallinity decreases and the lower glass transition of the quenched amorphous PPO appears [108], indicating that the RAF has actually a glass transition that lies above the zero-entropy-production melting temperature and the RAF keeps the crystals from melting and also prohibits reversible melting.

This behavior of the RAF, identified by TMDSC, has given a clearer picture of semi-crystalline polymers. One of the main features is the connection between the crystalline and the amorphous phase which was already observed in form of tie molecules and loose loops when analyzing crystal morphology[21], but had been largely neglected in explaining thermodynamic and mechanical properties. A better understanding and link between mechanical and thermal properties can now be expected, but it should vary for different types of flexible macromolecules.

(**e**) Besides the four major research directions in this time period from 1996 to 2003 just described, work continued on the expansion of the ATHAS Data Bank [82]. Data were collected for poly(oxy-1,4-benzoyl), poly(oxy-2,6-dimethyl-1,4-phenylene) (PPO), and poly(thiophenylene) [188]; poly-*p*-dioxanone, poly(trimethylene terephthalate), and poly(butylene terephthalate) [189]. A number of exact copolymers were also analyzed, which turned out to be of importance in the following research period, described in Section G [190]. Also of importance for this further work was the analysis of precise copolymers synthesized from large repeating units. Their mesophase structure could be probed by the crystallization behavior with quantitative thermal analysis, their motional characteristics, measured by solid-state NMR, and their crystal structure and morphology by X-ray diffraction [191].

The study of the poly(amino acids), their copolymers, and proteins [133, 134], which was described on page B-21 and illustrated with Figure 18, slowed after some additional work [192, 193]. The major effort it deserved could not be undertaken because of disinterest by the funding agency (see page 9-13). This research had to be continued using the unrestricted Distinguished Scientist support attached to my position at ORNL and UTK (see page 9-6), and was supplemented to some degree by the Polymer Program of NSF (as long as the proteins could be justified as

'polymers'). The results suggested the beginning of a glass transition in poly(L-methionine) and poly(L-serine) [193]. The behavior of the proteins is sufficiently similar to the synthetic polymers to deduce that there may also may be glassy nano phases imbedded in the overall structure and local areas of reversible structure-changes which now could be quantitatively investigated by TMDSC. The remaining step before linking the poly(amino acid) data [133] to native proteins is the evaluation of the changes of the partial molar thermodynamic functions with changing amounts of water. This step has been spearheaded by Dr. Pyda and is to be continued at the University of Technology in Rzeszow, Poland. Figure 30 illustrates the work on the heat capacity of dry starch. To get quantitative information on the hypothetical heat capacity of liquid starch, the prior data on glucose [75] were analyzed as shown on the left, and then used as an estimate for the right. Indeed, there is a clear beginning of a glass transition in starch at room temperature which, however, reaches only partial mobility. Two additional steps are introduced when water is added to the system [194].

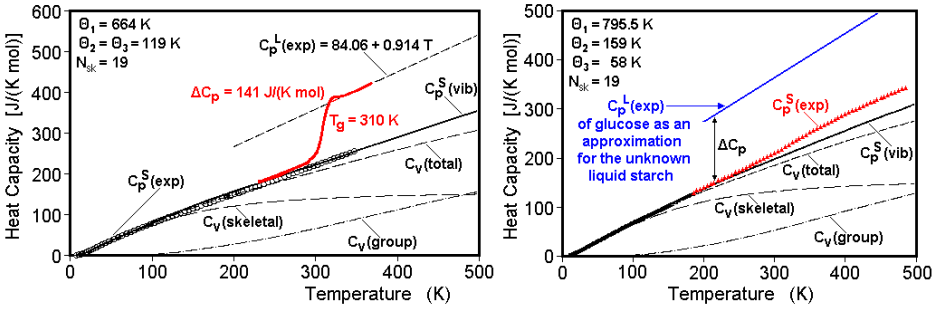

Figure 30 *Analysis of the heat capacity of glucose as model for starch (left), and data on dry starch, shown on the right, indicating the beginning of a glass transition at about 250 K.*.

The updating of the computation scheme for the ATHAS from the main-frame computer to the now sufficiently fast PCs is also listed in [85] and illustrated in Figure 18. The computation of the heat capacity of liquids has been further developed from the earlier, simple statistical model [86] to an adaption of the Ising model [195] to account for some degree of cooperativity shown by the large-amplitude, conformational motion in the liquid. Since these model calculations do not recognize a glass transition at low temperature, it was possible to extrapolate the C_p of polyethylene based on experiments from 250–600 K down to 0 K. Figure 31 shows the results [196]. Using the 'external' contribution to $C_p - C_v$, as determined from the liquid expansivity and compressibility, yields still an unreasonable residual entropy of -6.8 J (K mol)$^{-1}$ at 0 K. At the temperature where the conformational contribution reaches zero, the external contribution, however, must similarly reach a value close to zero, as known from the glass. Making this correction, a residual entropy of +0.41 J (K mol)$^{-1}$ is reached at 0 K, and the Kauzmann Paradox [197] is avoided. Note, that the free enthalpy at absolute zero is still large and positive, indicating the metastability of the liquid relative to the crystal. Its value of +2.1 kJ mol^{-1} is ≈50% of the enthalpy of fusion at T_m^o [196].

A nonequilibrium phase diagram of poly(4-methyl pentene-1) is shown in Fig. 32 [198]. It was derived from thermal analysis and structure data measured in the laboratory of Prof. Rastogi. Of particular interest is the difference to the phase diagram of polyethylene in Figure 6. While

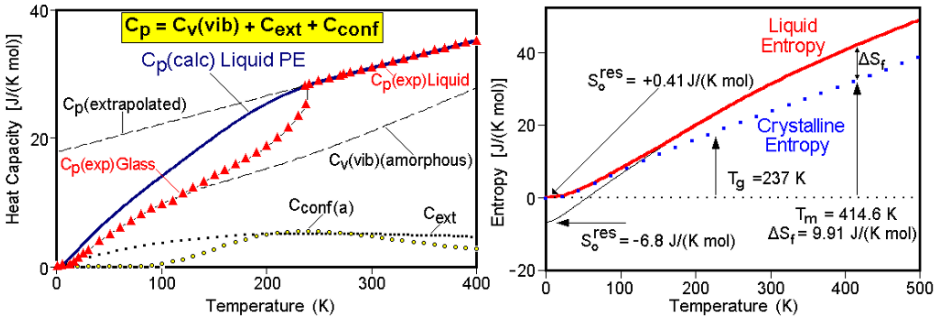

Figure 31 *Calculation of the heat capacity and entropy of liquid polyethylene to 0 K, omitting any glass-transition effects. The entropy remains positive to 0 K and shows no Kauzmann paradox.*

polyethylene possesses a stable condis phase at elevated temperature and pressure, poly(4-methyl pentene-1) exists only as a metastable phase below the glass transition. This is a behavior similar to that seen in polypropylene [103]. The condis glass is reversibly produced by isothermally increasing the pressure at room temperature and reverts on heating to the trigonal phase, as shown on the right side of the phase diagram. Also shown is the maximum in the melting temperature which is linked through the Clausius-Clapeyron equation to an inversion of the density difference between crystal and melt on increasing the pressure. A similar inversion occurs when cooling the crystals at atmospheric pressure, so that at room temperature, the crystal has a lower density than the melt [100].

New X-ray data were also generated for tetra-alkyl ammonium salts of small chain length (methyl and ethyl) [199] to support the earlier extensive analyses of the condis-crystal forming salts with up to octadecyl groups [123]. Another small molecule, a neopentane ester, was analyzed with respect to heat capacity, structure, and molecular motion [200]. Finally, the computation of the heat capacities of a series of oligophenylenes was carried out [201], and connected to the earlier calculations and discussions on phenylene-containing polymers [109].

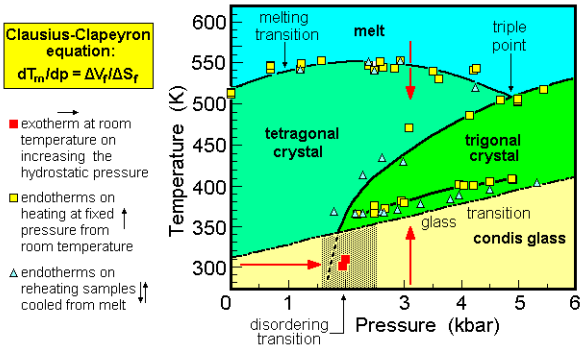

Figure 32 *Phase diagram of poly(4-methyl pentene-1).*

(**f**) A final topic during this time period dealt with the production and analysis of extremely small samples making an attempt to direct the research toward the analysis of nano phases. The work on separating single macromolecules on the liquid surface of a Langmuir trough and analysis by electron microscopy and diffraction [136] continued and was extended to electro-spray techniques followed by AFM observation [202]. Polyethylenes, poly(oxyethylene)s, atactic and

isotactic polystyrenes were analyzed as glassy spheres and single crystals (see Figures 43 of Chapter 9). Molten single-molecule droplets of isotactic polystyrene crystallize to a metastable, chain-folded single-crystal lamella and not to the expected equilibrium rod. Unfortunately, a technique to check the glass transition of the single-molecule glasses and the melting and annealing behavior was not available at this time, but will be described in the next section. An initial effort was made with a commercial microcalorimeter, but we could succeed only in analyzing thin, continuous films [203]. The limits of the AFM thermocouple were evaluated, and perhaps the next generation of tips for AFM (Figure 42 of Chapter 9) will be sufficiently small for a direct thermal analysis of nano phases, such as single-molecule particles [146]. An alternative, perhaps more likely to be successful in this task, is the chip calorimeter, to be described in Section G.

G. CHAIN SEGMENT DECOUPLING OF FLEXIBLE MACROMOLECULES (2001–2006)

With the retirement in 2001, the support through ORNL and UTK, which funded about half of the research effort was terminated. The NSF support, however, still continued until 2003, and when submitting an additional proposal, it was granted, lasting until 2006. The description of this work forms the core of this Section G. The laboratory was maintained at its old level under the direction of Dr. Pyda, and the physical upkeep was continued by both ORNL and UTK. Cooperation was kept with several of the former coworkers. From 2001–2006 about 70 papers and conference reports were contributed to the literature. It took until 2008 for final publication of the last research experiments. Beyond this time, there remains the capability to continue teaching the computer course on 'Thermal Analysis of Materials' [117] and to update it with news gained from the attended conferences on the topic, to consult via e-mail and during occasional visits, and, may be, to contibute to the solution of some of the old problems. It could also be, that there is time left for some private hobbies, sadly neglected over the past 25 years (see page 9-83).

The term *decoupled chain segments in nano phases* of parts of macromolecules were already mentioned in Sections C and F. The decoupled parts of long molecules must be described by different thermodynamic and mechanical functions. The points of decoupling may collect at phase boundaries. In copolymers, they may also mark the change in chemical structure. In amorphous, flexible polymers they also may be linked to points of entanglement. In chemical processes, the term coupling can also be used to describe the time sequence of successive reactions which may be a coupling between reversible and irreversible processes. The biological ADP to ATP conversion is a prime example. In macromolecular physical processes, a typical example are the phase transitions coupled to mixing or demixing. Depending on the relative rates they may be independent, sequential processes or occur simultaneously, as generally seen for small molecules.

Naturally, there are different degrees of coupling, as became obvious when studying the RAF. In fact, the attention to this concept had its beginning at the 1979 'IUPAC Symposium on Thermal Analysis' in Prague (see Appendix C, page C-21). After my lecture on 'Specific Heats of Linear Macromolecules,' a heated discussion about the change in C_p at the T_g of semicrystalline polymers put the additivity of C_p in doubt, and with it, the two-phase model. This discussion started investigations in our laboratory which led to a three-phase model [91, 92], with the RAF being partially coupled at the crystal interface. The coupling being caused by stress-transfer which creates an amorphous nano phase with a higher T_g than the bulk phase. This description of the phase structure, as well as the concept of decoupling, is expounded in [204].

As in each of the prior sections, experimental progress is to be reported first. After summarizing the advantages, and bemoaning the frequently less-than-quantitative thermal analyses in the literature, one of the old problems in the DSC of fibers and liquids was resolved [205]. It was found that on melting, drawn fibers will shrink with such force that the sample pan deforms. This also is true when cycling a sample between solid and liquid. The sample may then locate itself in the crevices of the cold-welded pan. A sample must be well isolated from the pan and given enough space to change its shape, or even not be taken through the solid-liquid transition to get the quality data of Figure 28. An example of this problem, is given in Figure 33. Higher precision could only be achieved by using two temperature ranges of calibrations for the first heating trace. First, at low-temperature, and then a second calibration beyond the melting peak. Subsequent cooling and heating, then, kept the second calibration. The deformations that the pans suffered are shown in the top insert of Figure 33. Only after this problem was solved, could the multi-frequency analysis of this fiber of ultra-high molar-mass polyethylene be completed [206]. (See also the discussion in Ref. [186].)

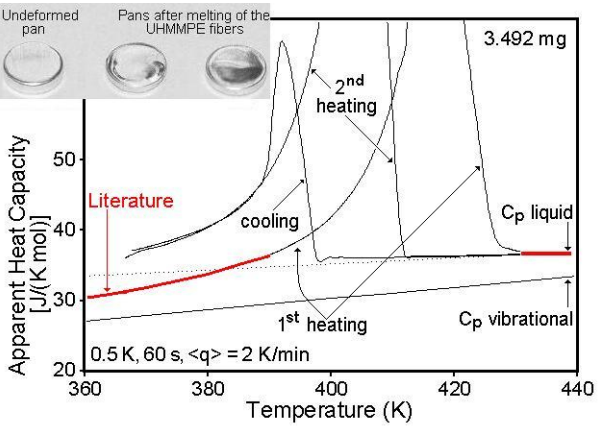

Figure 33 *Standard DSC of a gel-spun PE fiber with an initial double fit with literature data (red) before and after melting.*

The main progress in instrumentation, however, did not come from the traditional makers of calorimeters, but from the manufacturers of electronic chips capable of measuring temperatures on extremely small samples. The first successful calorimeters were summarized during the Lähnwitz Seminars in Germany in 2002 and 2004, and the 2004 NATAS Meeting in the US [207]. Our own effort on fast measurements were concerned with thermometry and DTA of the melting kinetics of polymer crystals and the possibility of identification of the metastable polypropylene mesophase [49, 50, 103]. In these experiments, rates of temperature change of almost 10,000 K min^{-1} were accomplished. From such experiments, it also became clear that samples of nanogram size could be heated with rates above 10,000 K s^{-1} with minimal internal temperature gradients. Such speeds were reached and exceeded with the super-fast chip calorimeters.

Experiments with an integrated chip thermometer (ICT) were performed in the laboratory of Prof. Schick on the samples also used in the measurements shown in Figure 29 and are displayed in Figure 34 [175]. Side and top schematics of the ICT are drawn as inserts. The PBT was quenched with about 10^6 K s^{-1} to the crystallization temperature with a coolant gas after melting in the ICT to produce an amorphous, liquid sample. The temperature change due to crystallization was then followed at the crystallization temperature (see the insert on the right). For slow analyses of quenched samples of PBT, see also the right graph of Figure 29. Of interest is the possible slowing of the crystallization rate by the glass transition of the RAF (compare Figure 29 and 43). No second

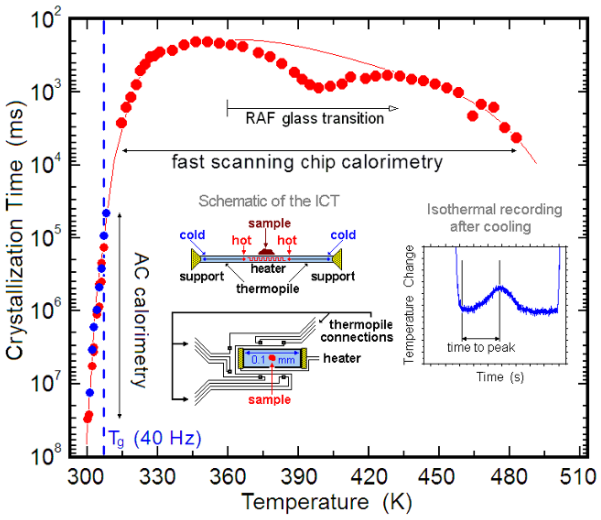

Figure 34 *Crystallization time of 0.1 μg PBT measured by ICT.*

crystal polymorph or change in crystal morphology is known for PBT to otherwise account for this observation.

The decoupling of crystal and surrounding amorphous material was studied with a wide range of POE samples [208]. Figure 26, above, contains the proof that the extended-chain crystals grown from sufficiently high-molar-mass samples, melt fully irreversibly. The same was found for sharply folded crystals, while with a molar mass above about 10,000 Da the behavior is that common for folded-chain crystals [144], and illustrated in Figure 26 for PET. When analyzing the thermodynamic C_p of POE crystals by quasi-isothermal TMDSC, it was found that it increased to the level of the liquid before melting, indicating a *glass transition of the crystal* [209]. This is presented in the upper left of Figure 35 and entered as a possible transition in Figure 13. The glass-transition temperature increased from about 310 K for the extended chain crystals of molar mass 1,500 Da to 324 K for crystals of molar mass above 20,000 Da. The X-ray data in the upper right of Figure 35 indicates no change in crystal structure up to the melt. The coherence length of the crystals, furthermore, stays constant and the unit-cell volume of the crystal increases normally up to the glass transition, and then shows an abrupt change in expansivity, as is commonly seen for glass transitions. Such behavior must drastically change the physical properties of the crystals. Normally, one would see under these conditions a disordering transition to a mesophase as shown in Figure 13.

The high mobility in POE crystals, however, is not unique, it is also observed in nylon crystals [131], where quasi-elastic neutron-scattering indicated liquid-like mobility [132] in parallel with an increase in C_p. These observations justify the definitions at the bottom of Figure 10. It is not the order in the crystal that makes it a solid, but the cooperative freezing of the large-amplitude motion at the glass transition temperature. Only as a secondary effect increases ordering the glass transition temperature, to coincide with melting. But in some cases there can be a glass transition within crystals below the melting temperature [210]. Isolated, large-amplitude motion has also been observed in crystals and causes the creation of equilibrium defects (see Figures 4 and 15).

The bottom-row of Figure 35 illustrates the most recent observations with TMDSC in the study of macromolecular crystals. Precisely constructed copolymers can be produced by special synthesis. Such copolymers melt as sharply as the homopolymers displayed at the top of Figure 26. The reversible, local melting of their crystals (monoclinic) is much less than seen for the random copolymers. The melting temperatures are close to the temperatures of melting of paraffins which

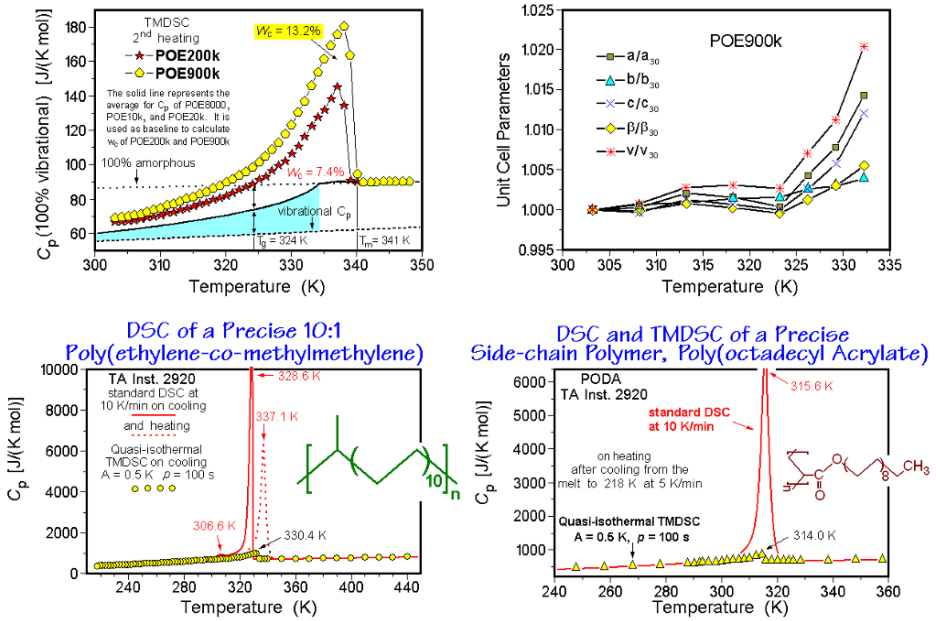

Figure 35 *Analyses by DSC, TMDSC, and X-ray diffraction. Top left: Apparent reversible heat capacity of POE indicating a glass transition of the crystals. Top right: X-ray data supporting a glass transition at 324 K. Bottom: Apparent reversible heat capacities of two precisely constructed copolymers. The left example has fixed sequences along the backbone, the right in the side chain.*

are comparable in length to the decoupled CH_2-sequences [210]. For the in-chain decoupled molecules in the left of Figure 35, the macroconformations, however, remain that of a macromolecule, as summarized in Figure 11, i.e., it is chain-folded at a length three times that of the CH_2-sequences. This is a result of the incomplete decoupling at the points of the change in chemical structure. The defects caused by these points of different chemical structure are collected in well-defined planes within the crystals and on the surfaces. Similar precise structures with larger interruptions were analyzed earlier. In these cases, the foreign units separating the CH_2 chains were aromatic sequences and separated as nano phases, also yielding an overall lamellar structure with multiple internal layers, closely coordinated in the mesophase structure [191].

Random copolymers behave quite differently. They were studied earlier and an example of similar CH_2-concentration and crystallinity as the precise copolymers is illustrated on the left in Figure 36 [172]. The DSC cooling trace, marked as the thin, continuous curve, shows a sharp peak of orthorhombic PE crystal growth, followed by a broad, hexagonal mesophase crystal growth. The DSC and TMDSC melting curves (dashed) prove supercooling on crystallization and start within the glass transition with much of the melting occurring reversibly.

Having examined a few examples from each of the full spectrum of molecules from oligomers to homopolymers and from homopolymers to random and precisely-engineered

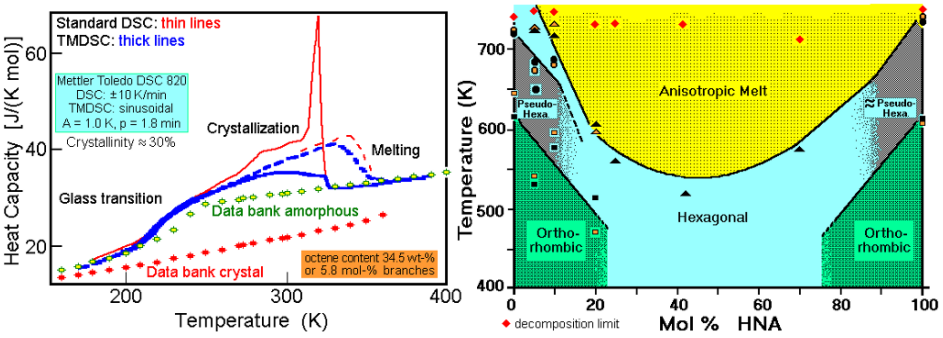

Figure 36 *Analysis of poly(ethylene-co-octene-1) with DSC and TMDSC (shown on the left), and the approximate phase diagram of poly(oxybenzoate-co-naphthoate) (shown on the right).*

copolymers, the breadth of the knowledge that needs to be collected to understand polymer crystallization became clear. For any material, such study is incomplete unless a detailed structure-property analysis is made over the temperature range of the transitions. In addition, a quantitative study of the reversible and irreversible thermodynamics is necessary to give information about the molecular motion within the different micro and nano phases and the coupling across the interfaces.

As during the earlier research periods, the effort to expand quantitative information for the ATHAS Data Bank was continued. The TMDSC of polytetrafluoroethylene was completed. The solid-solid transition of the triclinic crystals from a 2*13/6 to a 2*15/7 helix at low temperature was found to be irreversible, while the subsequent disordering at slightly higher temperature is reversible [211], and the transition from the trigonal condis crystal to the melt is similar to the melting of polyethylene [212], i.e., the melt-crystallized, folded-chain crystals show a certain fraction of locally reversible melting, while the extended-chain crystals, do not (see Figure 26 for PE and PET).

The specific RAF of cold crystallized poly(ethylene terephthalate), i.e., the ratio between the RAF and crystallinity at the glass transition temperature of the mobile-amorphous fraction was found to decrease from almost two, to 0.75 after annealing [213]. This decrease of the specific rigid-amorphous fraction is due to crystal perfection, i.e., an increased decoupling of the amorphous and crystalline phases. This should be compared to the even stronger coupling of PPO in Figure 26 (bottom left), where the RAF to crystallinity ratio was approximately three.

Another research update and completion involved the phase diagram of poly(oxybenzoate-*co*-naphthoate) which is illustrated at the right of Figure 36 [214]. Due to the similar overall shape of the repeating units, a mesophase-like order is seen in the center and high-temperature areas of the diagram. Only in the vicinity of the homopolymer compositions are true crystals observed. The earlier work on the calorimetry of this and similar other copolymer systems are described in [113].

A final ATHAS effort at UTK dealt with two biodegradable polymers, poly(lactic acid) and poly(vinyl methyl ether) [215]. For both, the thermodynamic functions and their interpretation were added to the Data Bank, and the reversibility was probed with TMDSC. This work broadens the work on the bio-related polymers, an effort continued by Dr. Pyda in his new location. Earlier work on biopolymers (starches and proteins) was already mentioned in Section F (pages B-34–35) and Section E (pages B-21–22).

H. FINAL PAPERS AFTER CLOSING THE LABORATORY (2007–2010)

Closing the laboratory in 2006, did not mean that all scientific work stopped. The main writing effort, started in 2007, involved the writing of my autobiography of the experiences and accomplishments in 20th Century Germany and USA (of which this Appendix B is a part [216]). The last experimental papers concerning polyoxyethylenes [208], poly(butylene terephthalate) [175], nylons [131], precisely constructed copolymers [210], and hydroxybenzoic acid copolymers [214]. They were completed and published between 2005 and 2008.

This left the writing of 14 general reviews and outlooks in specific fields to which modern thermal analysis contributes. Most of these were prepared in conjunction with scientific meetings which are listed in Appendix C along with two book chapters [224 and 229]. The breadth of topics can be seen from their titles:

➔100 Years Research on Supercooling and Superheating (9th Lähnwitz Seminar, 2006 [218])

➔Calorimetry of Nano Phases of Macromolecules (16th Symp. Thermophys. Props. Boulder, CO, 2006 [219])

➔The Use of Modern DSC for the Study of Metastastable and Unstable Materials [220]

➔Fifty-year Development of the Understanding of Motion and Defects in Macromolecular Crystals Based on Thermal Analysis Structure Analysis, and Computer Simulation (234th ACS Meeting, Boston, MA, 2007 [221] which brought together many of the researchers in this field as shown in Figure 37, see also page 10-8 and 8-63 for more details)

➔Thermal Properties of Aliphatic Nylons and Their Link to Crystal Structure and Molecular Motion (35th NATAS Conf. East Lansing, MI, 2007 [222])

➔The Differences in Structural and Thermal Properties Between Random and Precisely Structured Copolymers of Polyolefins (Meeting on Advances in Polyolefins, in Santa Rosa, CA, 2007 [223])

➔Thermodynamics and Kinetics of Crystallization of Flexible Molecules [221].

➔The Phases Between Solid and Liquid, Characterized by Thermal Analysis [224]

➔Temperature-modulated Calorimetry of Poly[oxy(benzoate-*co*-naphthoate)]s as Examples of Rotationally Hindered Polymers, (36th NATAS Conf., Atlantic City, GA, 2008 [225])

➔Thermodynamics and Properties of Nano Phases. (10th Lähnwitz Seminar, 2008 [226])

➔Quantitative Quasi-isothermal TMDSC Techniques To Separate Reversible and Irreversible Thermodynamic Changes in Heat Capacity in the Glass Transition and Melting Range (ICCT 08, Warszawa, Poland, 2008 [227])

➔Thermodynamic Description of Condensed Phases (37th NATAS Conference on Thermal Analysis and Applications, in Lubbock, TX, 2009 [228]

➔Thermal Analysis of the Condensed Phases [229]

➔Global and Local Phase/Molecular Nucleation, Solid/Mobil, and Order/Disorder Transitions in Macromolecular Systems. (To be based on a projected lecture to be given at the 11th Lähnwitz Seminar in Rostock-Warnemünde, June 6–11, 2010 [230]).

Figure 37

50th ANNIVERSARY SYMPOSIUM OF THE DISCOVERY OF POLYMER SINGLE CRYSTALS

Stephen Z. D. Cheng and Andrew J. Lovinger, Organizers

American Chemical Society Meeting, Boston, 19-22 August 2007

1: Darrell Reneker (U. Akron); **2**: Robert Prud'homme (U. Montreal); **3**: Phil Geil (U. Illinois); **4**: Gert Strobl (U. Freiburg); **5**: Bernard Lotz (ICS, CNRS, Strasbourg); **6**: Akihiko Toda (Hiroshima U.); **7**: Buck Crist (Northwestern U.); **8**: Haopeng Wang (Case Western); **9**: Rufina Alamo (Florida A&M U.); **10**: Rick Register (Princeton U.); **11**: Andy Lovinger (NSF); **12**: Bernhard Wunderlich (U. Tennessee); **13**: Christoph Schick (U. Rostock); **14**: Matthias Ballauff (U. Bayreuth); **15**: Peggy Cebe (Tufts U.); **16**: Hendrik Meyer (ICS, CNRS, Strasbourg); **17**: Kohji Tashiro (Toyota Tech Inst.) **18**: Daniel Alcazar (MIT); **19**: Ben Hsiao (SUNY Stonybrook); **20**: Hyun Hoon Song (Hannam U., Korea); **21**: Greg Rutledge (MIT); **22**: Jerry Schultz (U. Delaware); **23**: Lei Zhu (U. Connecticut); **24**: Lekshmi Kailas (U. Sheffield); **25**: Freddy Khoury (NIST, NSF); **26**: Ned Thomas (MIT); **27**: Dave Martin (U. Michigan); **28**: Rong-Ming Ho (National Tsing Hua U.); **29**: Stephen Cheng (U. Akron); **30**: Sanjay Rastogi (Loughborough U.); **31**: Claudio De Rosa (U. Naples); **32**: Tom Russell (U. Mass.Amherst); **33**: Julie Kornfield (Caltech); **34**: Peter Dias (Case Western); **35**: Chris Li (Drexel U.).

I. CONCLUSIONS AND ACKNOWLEDGMENTS

Over the last 50 years much progress has been made in the understanding and techniques of thermal analysis of polymers. My students and I were fortunate to be part of this development. Who could have predicted in the 1950s the possibility to visualize the thermal motion by supercomputer, the ability to make complete measurements of heat capacity in less than a day, the ease with which the heat capacity of proteins can be computed from its thousands of normal mode vibrations, to estimate quantities for which there are no theoretical correlations (as yet) *via* neural net calculations, to separate reversible and irreversible processes by calorimetry, and to make measurements on nanograms of material at rates as fast as one million kelvin per second? Finally, it was difficult to imagine that 50 years later, it is possible to disseminate this advanced thermal analysis system over the internet and study the material anywhere in the world where there is an internet connection.

Thermal analysis and polymer science have changed and grown, becoming evermore exciting. Thermal analysis is one of the fastest growing experimental and theoretical research tools and further developments are expected, permitting increasingly more quantitative measurements on smaller sample sizes. Polymers science brings forth increasingly more precise synthetic molecules of special design which ultimately may reach the complexity of biopolymers, so that modern calorimetry will increasingly be able to contribute to the understanding of all macromolecules [231].

For General Acknowledgments see the Front Material of the book. It should be remembered that all topics mentioned in this Appendix B are linked in great detail to the literature in the many hundreds of references cited in the pertinent reviews [11, 45, 52, 54, 61, 62, 94, 143, 144, 218, 231], books [21, 93, 116], and the computer course [117]. Last, but by no means least, I would like to thank Dr. E. Turi for the invitation to write the first version of this Appendix B (see Footnote, page B-1) and for her untiring effort to entice so many of my students and friends to contribute to the 65th birthday issue of the Journal of Thermal Analysis (see page 9-18), and Dr. J. Menczel, who arranged the 75th birthday symposium at the 34th NATAS Meeting and the printing of the second version (see page 10-8 and the Footnote, page B-1). Finally, all was updated and fitted as part of this book [216], arranged to be published by Springer, Berlin (see Footnote, page B-1).

J. REFERENCES

(Numbers without brackets within a Reference point to work from our laboratory and refer to the list given in Appendix A. Multiple listings under one reference contain all participating authors, but not every listed author is necessarily a coauthor in each of the papers of the group of publications. Titles and citations need to be looked up in Appendix A, information about Meetings in Appendix C.)

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[220]. 576. B. Wunderlich.
[221]. 577, 581. B. Wunderlich.
[222]. 578a,b. B. Wunderlich.
[223]. 579. B. Wunderlich.
[224]. 582. B. Wunderlich.
[225]. 583. B. Wunderlich; see also [214].
[226]. 584. B. Wunderlich.
[227]. 585. B. Wunderlich.
[228]. 586a,b. B. Wunderlich.
[229]. 580. B. Wunderlich.
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Appendix C

Permanent Homes, Travel, and Lectures of Bernhard Wunderlich

Permanent Homes are in bold-face, travel and temporary homes are indented. Listed are the numerous lectures outside the scheduled lectures at the home university. Contributions listed under the names of coworkers were presented by the first listed person. An * before the presenter indicates that the lecture was given by a coworker who attended the indicated meeting in absence of Professor Wunderlich. Major private travel after 1954 with no or minor professional presentations is listed under a separate heading as Part C of this Appendix. Temporary changes in places of residence, such as during sabbatic leaves are within the bolded brackets **[ ]**. Trans-Atlantic, trans-Caribbean, and trans-Pacific travel, as well as more extensive lecture series, are given under separate headings.

A. GERMANY (1931–1954)

1931–1945 ***Brandenburg an der Havel*** **(until 1933 Weimar Republik, then "3. Reich.")**
(Chapter 1, Figures 5 & 6; Chapter 2, Figures 6 & 12; and Chapter 9, Figure 26.)

1931 Wilhelmsdorfer Straße 70
(First home I remember; to ≈1934 fourth floor, then first floor.)

1936 Travel by car to Landsberg an der Warthe to visit relatives (see page 1-9).
Christmas vacation in Lautenthal/Harz.
1937–39 Summer and Christmas vacations in Lautenthal/Harz (see pages 1-8, 9, 23, 2-3, 8-50 and Chapter 1, Figure 10).
1938 Additional travel by train/car to Rüsselsheim/Rhein, to pick up Vati's new car (see page 1-26 and Chapter 1, Figure 23).

Begin of WWII, stop of most vacation travel.

1940 Visit to Tante Grete and Oma in Stralsund on the Baltic Sea (see page 2-3).

1941 Werderstraße 28
(Former orphanage, now four apartments, garden, business yard, see pages 2-10–11.)

1941 Enter the "Theodor von Körner Mittelschule" (middle school, see pages 2-4–5).
1942 Summer, convalescence in Bad Mergentheim (see page 2-16).

1943 "Kinderlandverschickung" to Rabka, Poland, 7 months (see pages 2-20–22).
1945 From about April 1, refugee, Krahne, near Brandenburg (see page 2-26).
April 20, our house was bombed, a total loss (see Chapter 2, Figure 9).
April 24, the Soviet troops reach Brandenburg.

Lindau/Elbe, refugees, May 1 to about 15th (see Chapter 2, Figures 14 and 15).

May 8, end of WW II

Lütte, bei Belzig, (about 2 months), refugees (see pages 3-1–4, Chapter 3, Figure 2).

1945–1949 Brandenburg an der Havel (Soviet-occupied Zone of Germany)
(Chapter 3, for the destruction in Brandenburg see Chapter 2, Figures 9 & 17–28).

1945 Hohenzollernstraße 11
(The family business remained in the Werderstraße, see Chapter 2, Figure 7.)

1945 Resume schooling at the "Theodor von Körner Mittelschule," and shortly thereafter begin work in the family roofing business for about 4 months due to difficulties to reach the school (see page 3-7).

1946 Franz-Ziegler-Straße 35
(Closer to the business and larger apartment, see Chapter 3, Figure 5.)

1946 Continue to attend the "Theodor Körner Mittelschule," then, on "School Reform," attend highschool in the same building with some of the same teachers (see Chapter 2, Figure 4 and Chapter 3, Figure 8).
1949 Graduation from "Johann Wolfgang von Goethe Oberschule" ("Abitur") and application to the Humboldt University, HU, Berlin (see Chapter 4, Figure 1).
1949 September 13 to November 9, 18 trips to Berlin and one to Greifswald to attain admission to a university for the study of chemistry.

1949–1953 Berlin (German Democratic Republic, GDR)
(Chapter 4, for the effort to gain admittance to the HU, see pages 4-1–8.)

1949 Am Friedrichshain 10, Landlady: "Fräulein M. Schmidt" (from November 1949). From the Winter Term 1949/50, student of chemistry at the Humboldt University (stud. rer. nat.), during the academic year, weekly trips between Berlin and Brandenburg (see pages 4-1 and 3).

1952 Easter, (April 13–15) short vacation in the Harz Mountains in Treseburg/Bode, Lautenthal (1936–39) was now in West Germany and off-limit to us (see page 4-24). Vacation in "Wendoche, bei Belzig" (see Chapter 4, Figures 16–18, page 4-24).
1953 Refugee, from June 17, 1953. First in West Berlin, Rudow (see Preface), then evacuated by plane to Frankfurt, continued by train to camp Weinsberg, near Heilbronn, FRG, "in Baden-Württemberg," (page 4-35, Chapter 5, Figures 1and 2).

1953–1954 Frankfurt am Main (Federal Republic of Germany, FRG)
(For details of Frankfurt, see text and Figures 10 and 11 of Chapter 5.)

1953 Refugee Camps First in camp Weinsberg from August (see Chapter 5, Figure 1), then, refugee camp Griesheim/Frankfurt until Nov. 1953 (see Chapter 5, Figures 5–6). Multiple vacation employments at the "Farbwerke Höchst," Frankfurt-Höchst, from 9/1953 to 9/1954. (The combined days were equivalent to about five months of work, see Chapter 5, Figure 7.)

1953 Trip from Weinsberg to Frankfurt for university admission, and later to move there.

1953 Mendelssohn Str. 81, (Chapter 5, Figure 8). Student, Goethe University (pages 5-3, 11, 12).

1953 December, trip to Werbach an der Tauber, the new home-town (see Chapter 3, Figure 31, pages 3-36 and 5-13).
December 28, married in the Römer in Frankfurt; followed by a three-day honeymoon in "Königstein am Taunus" (see Chapter 5, Figures 16–21).
1954 October 26, sailed from Bremerhafen on the Gripsholm for New York City, USA.

B. UNITED STATES OF AMERICA (from November 1954–)

1954–1955 Hastings, Nebraska
(Chapter 6, pages 6-1–17; travel to the US, pages 5-18–22; Hastings College, pages 6-3,5)

Arrival in New York City on 11/6, 1954, with the ship MS Gripsholm (North German Lloyd), later renamed to MS Berlin. Further travel with the 'Broadway Limited' from New York City, NY to Chicago, IL and then with the 'Denver Zephyr' to Hastings, NE, to arrive there on November 7 at 3 a.m. Initial stay with "Tante Lieschen" at 212 N 12th Street. From the middle of the Fall Term, admitted as student to Hastings College. (Worked at Ingleside State Psychiatric Hospital as a ward attendant in the afternoons and evenings.)

1955 113 East 4th Street (see Chapter 11, Figure 42) rented in January from Mrs. Mizen.
(Spring Term, student at Hastings College and applications for graduate study. Gained assistantship to Northwestern University in Evanston, IL, for the Fall Term 1955.)

1955–1958 Chicago, Illinois
See Chapter 6, pages 6-17–38. Northwestern University (see pages 6-13, 14 and 23).

1955 7729 North Sheridan Road (We rented an efficiency apartment, see Chapter 11, Figure 23.) Beginning with the Fall Term: Graduate student of chemistry at Northwestern University, Evanston Illinois (Dr. Malcolm Dole, Research Director); annual travels back to Hastings NE by car (650 miles), usually at Christmas time; travel by car to Toronto, Canada in 1958.

1957 Summer, PhD Exam after four semesters and two summers of research and study.
Fall Term: Appointment as Instructor of Chemistry at NU until August 31, 1958.

1957/58 *Interview Trips, lectures on Cold Crystallization of High Polymers:* (page 6-35). Union Carbide, Visking Company, Chicago, IL, September 10, 1957; Loyola University, Chicago, October 1, 1957; General Electric Company, Schenectady, NY. February 7, 1958; Union Carbide, Headquarter in New York City and the Bakelite Company in Bloomfield, NJ, February 27–28, 1958; Cornell University, Ithaca NY, March 11, 1958; University of North Carolina, Chapel Hill, NC, March 17, 1958; DuPont de Nemours in Wilmington, DE and Parlin, NJ, March 24–26, 1958; Eastman Kodak Company, Rochester, NY, March 27, 1958; Shell Development Company, Emeryville, CA, April 10 and 11, 1958 (in conjunction with a lecture at the Spring ACS Meeting; in San Francisco, CA, April 13–17). Illinois Institute of Technology, Chicago, IL, May 6, 1958. (See also the pages 6-34–37.)

1958–1963 Ithaca, New York
(Chapter 7, for information on Cornell University, see pages 7-2 and 3)

1958, 18 Hawthorne Circle, rented a duplex, Chapter 7, Figure 1. Additional annual travel back to Hastings NE by car (≈1300 miles one way), usually at Christmas time.

1958 Start as Instructor at Cornell University for the Fall term 1960. From the Spring term 1963, Assistant Professor of Chemistry.

1959–61 ACS, IUPAC, and other lectures. The additional lectures were not recorded in detail until approximately 1963. From then on. annual reports were filed. These and other trips involved usual travel by car and went to NYC, Philadelphia, Buffalo, Rochester, Detroit, Toronto, Montreal, and 30 times to teach at Harpur College in Binghamton, NY (described on page 7-5).

1962 *Contract as exclusive consultant for DuPont de Nemour and Co.* (see page 7-5). First, at the Electrochemicals Division in Niagara Falls, NY, 10 day-long presentations on "Mechanical Properties of Polymers," followed by dicussion and consultation. Later, additional visits to other plant and research facilities in Waynesboro, VA (Textile Fiber Dept., Benger Lab.); Parkersburg, VA (Textile Fiber Dept.); Martinsville, VA (Nylon Technical Div.); Circleville, OH (Film Dept.); Kinston NC (Dacron Research Lab.); Buffalo, NY (Yerkes); Orange, TX (Sabine River Works, Plastics Dept.); Richmond, VA (Spruance Film Research and Development Lab.); Philadelphia, PA (Marshall Lab, Fabrics and Finishes Dept.); Seaford, DE (Photo Films); and (in the later years almost exclusively) to the Central Research Station in Wilmington, DE (Textile Fibers Dept.; Engineering Dept.; Fabrics and Finishes, F&F Dept.; Electrochemicals Dept. at the Experimental Station and Chestnut Run locations; Plastics Dept.; Central Res. Dept.; Elastomers Dept.; Instrument Div.; Legal Dept.); finally, also to DuPont Canada (Montreal, legal advice on PE pipe failure). In total, ≈250 days were spent consulting and functioning as expert witness in legal proceedings from 1962 to 1988. Many visits included an informal lecture on research topics from our laboratory, the formal, invited lectures are listed below with their details.

1962, cont. Thermal Motions in Solid High Polymers. Invited lecture at the first Biennial Symposium of the American Chem. Soc. Polymer Div., East Lansing, Michigan, June 20–22 (see Chapter 7, Figure 30 and page 7-22).

Crystallization of Polyethylene under Elevated Pressure. Paper contributed to the Meeting of the American Chem. Soc. in Atlantic City on September 9–14.

The Defect Structure of Highly Crystalline Polyethylene. Paper contributed to the American Chem. Soc. in Atlantic City on September 9–14.

1963 Polymer Melting. Discussions at the Winter Gordon Conference in Santa Barbara, CA, February 4–8.

Polymer Crystallization at Elevated Pressure. General Discussion contributed to a meeting at the Watervliet Arsenal, Watervliet, NY, March 14–15.

Primary and Secondary Transition Intervals in Amorphous Polystyrene. Lecture at the American Phys. Society March Meeting in New York, NY, March 25–29.

1963–1988 Troy, New York

(See Chapter 8, employment at Rensselaer Polytechnic Institute, see pages 8-1 and 8-20.)

1963, 211 Winter Street. Extension, village of Wynantskill (zip: 12180, see Chapter 8, Figure 2) (June, 1963 Associate Professor of Chemistry, followed by promotion to Full Professor in 1965, and early retirement as of January 1, 1988). During these 24½ years there were five sabbatic or similar leaves. Two in Germany, the first (1967/68) was helped by financial support through my research grants and the University of Mainz (see the pages 8-37–51). The work dealt with "Crystallization during Polymerization," (publ. 61); the second sabbatic in Germany (1986/87) was supported partially by RPI and the University of Freiburg and to this were added the financial reward connected with the Humboldt Prize. The sabbatic was at the Universities of Freiburg and Ulm and had the goal to investigate the topic "Conformational Motion and Disorder," as found in condis crystals, (publ. 263) (see also pages 8-115–123). The three leaves in Troy were in 1970/71 and 1973/74 (connected with the writing of "Macromolecular Physics," (publs. 95, 102, 123) and in 1980/81 one semester was spent on recording and writing of the audio-course on "Thermal Analysis," (publ. 184). These five leaves also permitted more extensive traveling during the respective years.

During the years at RPI, monthly or more frequent consulting trips were taken to various laboratories of the DuPont Co. (see page C-4). Our private trips and vacations were, whenever possible, connected to the conference and lecture sites (see pages 8-36 and 37), and naturally, the usual trips by car to Hastings NE and the visits with various friends in the north-east were continued. Our favorite vacation spots are listed on pages 8-49–51.

1963, cont. (A) DDTA of the Glass Transition Interval. (B) Irreversible Melting of Polyethylene Copolymers Investigated by Differential Thermal Analysis. Lectures at the Fall Meeting of the ACS in New York, NY, September 8–13.

The Irreversible Melting and Dissolution of Metastable Polymer Crystals. Invited lecture at the 56th Annual Meeting of the Am. Inst. of Chemical Eng. in Houston, TX, December 1–5.

1964 (A) Comparison of Polyethylene and Asbestos Morphology. (B) P. H. Geil, The Morphology of Polyethylene Crystallized from the Melt under Pressure. Two contributions to the American Physical Society Meeting in Philadelphia, PA, March 23–26.

Polymer Crystallization. Participant at the Second Biennial Symposium of the Am. Chemical Society in Durham, NC, June 22–24, and the Discussions in the Polymer Gordon Conference at New London, NH, July 6–10.

The Melting of Defect Polymer Crystals. Contributed lecture to the 148th Am. Chem. Soc. Meeting in Chicago, August 30–September 4.

Crystallization of Macromolecules. Participant in the General Electric Professors Conference in Saratoga, NY, September 8–11.

1965 Melting of Linear High Polymer Crystals. Invited speaker at the 10th Intercollegiate Chemistry Program at the State University of Albany, March, 13.

Thermodynamics of the Melting of Polymer Crystals. Invited paper at the Am. Phys. Soc. Meeting in Kansas City, MO, March 24–27.

Thermodynamics of Crystalline Linear High Polymers, The Melting of Copolymers. Invited Lecture at the Am. Chem. Soc. Meeting in Detroit, MI, April 4–9.

First trip from the US to Europe (Germany) with family (See also page 8-22.)

Das Kristallisieren und Erstarren von linearen Hochpolymeren. Plenary lecture at the Kunststofftagung in Lübeck, Germany, May 3–6.

Melting of Linear Macromolecules. Seminars at the University of Mainz, Germany, May 10, the University of Marburg, Germany, May 12 and at the German Kunststoff Institut, Darmstadt, Germany, May 15.

Das Schmelzen von Hochpolymeren. Lecture at the Research Laboratory of the BASF, Ludwigshafen, Germany, May 17.

Differential Thermal Analysis of Linear Macromolecules. Invited lecture, Gordon Conference on Analytical Chemistry, New Hampton, NH, Aug. 8–13. (For the general information on Gordon Conferences, see pages 8-16, 17, 22.)

Second trip to Europe to the IUPAC and ICTA Meetings (See page 8-22, 23.)

Crystals of Linear Macromolecules. Invited lecture at the Polymer Institute of Hungary in Budapest, August 27.

Thermodynamic Properties of Extended Chain Polymethylene Single Crystals. IUPAC Symposium lecture in Prague, Czechoslovakia, September 1–5.

Thermal Analysis of Crystalline Polymers with Extended Chain Conformation. Lecture at the first ICTA-meeting in Aberdeen Scotland, September 6–10.

Superheating of Linear High Polymer Crystals. Invited lecture at the Cellulose, Wood and Fiber Division, at the 150th Meeting of the Am. Chem. Soc. in Atlantic City on September 12–17.

1966 Instruction and Research in Polymer Science at Rensselaer Polytechnic Institute. Lecture at a Symposium on Education in Polymer Science, University of Massachusetts, February 26.

1963, cont. (A) Initial Growth of Polyethylene Crystals. (B) Zone Polymerization of Caprolactam to the Crystalline State. (C) Melting of Equilibrium Crystals with Broad Molecular Weight Distribution. Three contributed papers to the Meeting of the Am. Phys. Soc., Durham, NC, March 28–31.

First Travel to Japan (With Heidel, ACS Charter flight, see pages 8-25–30.)

Melting of linear macromolecules. Lecture at the research laboratories of Teijin Co. at Osaka, Japan, September 17.

Melting and Structure of Extended Chain Crystals of Polyethylene. Seminar at the University of Fukuoka in Fukuoka, Japan, September 19.

Surface Structure and Melting of Extended Chain Crystals. Seminar at the Tokyo Institute of Technology, Tokyo, Japan, September 23.

Melting of Macromolecules. Lecture at the University of Tokyo, Tokyo, Japan, September 27.

(A) T. Davidson, Crystallization and Thermal Analysis of Extended-chain Ethylene Copolymers. (B) The Equilibrium Melting of Polymers. Two lectures at the IUPAC Symposium in Kyoto and Tokyo, Japan, September 30.

Extended Chain Crystals of Linear High Polymers. Lecture at a Polymer Meeting at the University of Osaka, Japan, October 5.

1967 *Lecture tour for the Am. Chem. Soc. (Atlantic Seaboard/Palmetto Circuits) from January 10 to 27* (See also pages 8-38 and 39.)*:*

A New Look at Polymer Melting. Invited lecture at the local ACS Meeting of the North Carolina Section, Raleigh, NC, January 10.

Extended Chain Polymer Crystals. Invited lecture at the DuPont Research Laboratories in Kingston, NC, January 11.

A New Look at Polymer Melting. Thirteen invited lectures at the local ACS Meeting of the (A) Hampton Roads Section, Norfolk, Virginia, January 12; (B) Virginia Section, Hopewell, Virginia, January 13; (C) Virginia Blue Ridge Section, Roanoke, Virginia, January, 14; (D) Central North Carolina Section, Greensboro, NC, January 16; (E) Carolina-Piedmont Section, Charlotte, NC, January 17; (F) Western Carolina Section, Brevard, NC, January 18; (G) South Carolina Section, Hartsville, SC, January 19; (H) Florida Section, Tallahassee, Florida, January 20; (I) Gainesville Subsection, Gainesville, Florida, January, 23; (J) Orlando Subsection, Orlando, Florida, January, 24; (K) Brevard Country Subsection, Cocoa Beach, Florida, January 25; (L) Tampa-Bay Subsection, Tampa, Florida, January 26; (M) Miami Subsection, Miami, Florida, January 27.

(A) F. Liberti; Melting of Nylon 6 as a Function of Morphology. (B) L. Melillo, Surface Recrystallization of Extended Chain Polyethylene. (C) M. Jaffe, Melting of Polyoxymethylene as a Function of Morphology. (D) F. Hamada, Density of Folded Chain Polyethylene Single Crystals and of Crystalline Hexatriacontane. (E) T. Davidson, Crystallization and Melting of Polymers under Pressure. (F) D. Hansen, Repeated Cold Drawing of Polymers. Six

contributed lectures at the March Meeting of the American Physical Society, Chicago, Illinois, March 27–30.

1967, cont. Discussion leader at a Conference on Structure and Mechanical Properties at the US Army Natick Laboratories, Natick, MA, April 19–21, 1967.

Electron and Interface Microscopy of Extended Chain Polymer Crystals. Invited lecture at the 8th Symposium on Polymer and Fiber Microscopy, Media, PA, May 18–19.

Superheating of Polymer Crystals. Thermal Methods Conference at the DuPont Company, Wilmington, Delaware, May 23–24.

Time Dependence of Specific Heats. Short Course on Differential Scanning Calorimetry at the University of Massachusetts, Amherst, MA, August 9–11.

[1967/68 First Sabbatic, in Germany, (six months leave with family, September 25 to March 29 to work on 'Cystallization during Polymerization' and give a course with weekly lectures on Thermal Analysis of Linear Macromolecules at the University of Mainz, see pages 8-37–49.)

Mainz/Kastell, Germany, Am Pionierübungsplatz 7 (bei Familie Siebert, Chapter 8, Figure 49)

1967, cont. Beweglichkeiten in kristallinen und amorphen Polymeren aus kalorischen Messungen. Invited lecture at the Discussion Meeting of the German Physical Society in Garmisch, September 27–29 (see page 8-39).

International discussion at the University of Mainz with participants of the German Physical Society in Garmisch, Oct. 4–5. [Drs. Hoffmann (NBS), Keller (University of Bristol), Lindenmeyer (Res. Triangle Inst.), Nöther (Chemstrand), and Keith (Bell Labs.); Stuart, Fischer, Schultz, and Meyerhoff (Mainz); Wunderlich (RPI), and coworkers and students of the University of Mainz.]

Specifische Wärme von Hochpolymeren (aus Differentialthermoanalyse als Messtechnik), "Antrittsvorlesung" at the University Mainz, on October 9. (Continued as a two-hour lecture each Thursday, for a total of 15 for the 68/68 Fall Term).

Diskussion von Wärmekapazitäten mit Dr. Baur of the BASF Ludwigshafen, visiting in Mainz, October 13.

Kalorische Messungen an amorphen und kristallinen Hochpolymeren. Two invited lectures at the Technical University in Clausthal, Harz, Oct. 20–21.

Kristalle von Hochpolymeren. Invited lecture and discussions at the Farbwerke Höchst, near Frankfurt, November 24. (with Dr. Wilski).

Kalorische Messungen an amorphen und kristallinen Hochpolymeren, lecture at the RWTH Aachen, November 27.

Diskussion von Wärmekapazitäten, Bayer AG, Leverkusen, Nov. 28. (Dr. Bonart).

Travel back to the US, Dec. 1–16. Spending one week at the DuPont Co, lecturing and consulting on High Polymer Research in Germany (travel to Wilmington, DE, Richmond, VA, and Circleville, OH). Dec. 11–15.

1967, cont. Diskussion von Wärmekapazitäten, Farbwerke Höchst, Dec. 22. (Dr. Wilski).

1968 Gestrechtkettige Kristalle von Hochpolymeren, Invited lecture and discussion at the Research Laboratories of Bayer AG, Leverkusen, January 12. (Dr. Bonart).

Kalorische Messungen an amorphen und kristallinen Hochpolymeren. Invited lecture at the Farbwerke Höchst, Frankfurt-Höchst, January 18.

Kristallisation von ungefalteted Ketten von Hochpolymeren. Invited lecture at the BASF, Ludwigshafen, Germany, Ludwigshafen, January 24.

Gestrecktkettige Kristalle. Lecture at the Meeting of the Gesellschaft Deutscher Chemiker, in Frankfurt, Main. January 25.

Kristallisation während der Polymerisation. Lecture and discussions at the University Marburg, January 29–30. (Prof. Müller, and Dr. Kilian).

Crystallization of Linear Macromolecules With and Without Chain Folding. Invited lecture at the Chemische Werke Hüls, Marl, February 9.

Polymerkristalle ohne Kettenfaltung. Kristallisation während der Polymerisation. Two invited lectures at the Max Planck Gesellschaft, Berlin, February 20–21.

Kalorische Messungen an amorphen und kristallinen Hochpolymeren. Invited lecture and general discussions at the Bundesanstalt für Materialprüfung, Berlin, February 22. (Prof. Becker).

Polymerkristalle ohne Kettenfaltung. Invited lecture at the Deutsche Akademie der Wissenschafter (of the GDR), Faserstoff Institut Teltow, Teltow, near Berlin, February 23. (Arranged by Dr. Ruscher)

Entwicklung der Polymerchemie in Deutschland in der Zukunft, Discussion at the University of Karlsruhe, February 28. (Arranged by Profs. Buckel and Volmert).

Polymerkristalle mit und ohne Kettenfaltung. Invited lecture, Macromolecular Colloquium, University of Freiburg, February 29–March 2. (Prof. Cantow).

Polymerkristallisation. Invited lecture at Bayer, Dormagen, on March 5.

Crystallization With and Without Chain-folding. Invited lecture and discussion, at the University of Strasbourg, France, March 6–7. (Arranged by Profs. Kovacs, Lotz, and Wittman).

Discussion of Polymer Research at the National Physics Laboratory in Teddington, England, March 11. (Dr. M. Richardson).

General Aspects of Polymer Research, University of Bristol, Bristol, England, March 12–13. (Arranged by Profs. A. Keller, F. C. Frank, and students).

Crystallization during Polymerization. Informal lecture and discussions of polymer research. Oxford University, Oxford, England, March 14.

Discussion of Polymer Research at ICI, Welwyn Garden City, England, March 15.

Simultane Polymerisation und Kristallisation. Final Colloquium at the University of Mainz, March 19.

Polymerkristalle mit und ohne Kettenfaltung. Plenary Lecture at the Spring Meeting of the German Physical Society in Gießen, March 26–28.

End of the First Sabbatic.]

1968, cont. Polymer Crystal Morphology. Lecture at the Second Symposium of the Annual Great Lakes Conferences on Polymer and Colloid Science, Norwood, Michigan, June 6–8.

Superheating of Extended Chain Polymer Crystals. Contributed lecture at the 2nd International Meeting of the ICTA, Worcester, MA, August 18–23.

Equilibrium Melting of Polyethylene. Lecture, IUPAC International Symposium on Macromolecular Chemistry, in Toronto, Canada, September 3–6.

Heat Capacities of Solid Polymers. Lecture at the Am. Chem. Soc. in Atlantic City, New Jersey, September 8–13.

Inorganic and Organic Glasses. Invited lecture at the First Northeast Regional Meeting of the Am. Chem. Soc. in Boston, MA, October 13–15.

Polymer Crystallization. Discussion contribution to the Sixth Cellulose Conference at the College of Forestry at Syracuse University, Syracuse NY, on October 14–15.

Differential Thermal Analysis. Lecture and discussion at the Seminar on Instrumental Chemical Analysis of the State Technical Services Program at Rensselaer Polytechnic Institute, November 7–8.

1969 Polymers, their Chemical Structure and Molecular Architecture. Seminar Lecture on the Polymer Science for Plastic Users at Rensselaer Polytechnic Institute, Troy, NY, January 26–27.

Theoretical Calculation of Thermodynamic Properties from Molecular Motion Parameters. Invited lecture at the Wayne State Polymer Conference, Detroit, MI, March 4.

Crystallization and Melting of Polymers. Symposium on the Thermodynamic Properties of Bulk Polymers at the US Bureau of Standards, Washington, DC, March 10–12.

(A) Reasons for Lamellar, Fibrous, and Spherulitic Habits of Linear High Polymers. (B) S. Wolpert, Dynamic Differential Thermal Analysis of the Glass Transition. (C) L. Melillo, Comparison of the Morphology of Extended Chain Crystals of Polytetrafluoroethylene and Polyethylene. Three Contributed lectures at the Am. Phys. Soc. Meeting in Philadelphia, PA, March 24–27.

Equilibrium Crystals of Polymers. Invited lecture at the Polymer Conference Series at the University of Detroit, Detroit, MI, May 22.

Crystallization during Polymerization. Invited Lecture at the Gordon Conference on Polymers in New London, NH, June 30–July 4.

ACS Charter flight to the IUPAC meeting in Budapest
(With Heidel, August 10–31, see pages 8-31–32.)

The Solid State of Linear Macromolecules. A lecture at the Research Laboratory of Bayer AG, Leverkusen, Germany, August 12.

Crystallization and Melting of High Polymers. Discussion at (A) the University of Marburg, Marburg, Germany, August 14, and (B) the University of Mainz, Mainz, Germany, August 18.

1969, cont. The Solid State of Linear High Polymers. Lecture at the Farbwerke Höchst, Frankfurt-Höchst, Germany, August 19.

Thermal Analysis of Polymers. Lecture at the BASF Research Laboratories, in Ludwigshafen, Germany, August, 20.

Crystallization and Melting of High Polymers. Lecture at the University of Freiburg, Freiburg, Germany, August 21.

Crystallization during Polymerization. Invited lecture, IUPAC Macromolecular Symposium, Budapest, Hungary, August 24–31.

Thermal Analysis. Lecture at the Program Design short course on Introduction to Polymer Science and Engineering, New York, NY, October 14.

Single Crystals of Linear High Polymers. Seminar at Cornell University, Department of Chemical Engineering, Ithaca, NY, October, 26.

1970 Morphology of Extended Chain Crystals. Lecture at the Firestone Company Research Labs, Akron, OH, January 15.

Thermal Analysis of Polymers. Lecture at the local ACS section in Akron, OH, January 16.

Crystallization in Copolymers of Linear Macromolecules. Lecture at the Research Laboratory of the Textile Fibers Department of the DuPont Company, Waynesboro, VA, January 21.

The Solid State of Linear Macromolecules. Lecture at the Chemistry Department of Clarkson College of Technology, Potsdam, NY, February 12.

DTA of Polymers. Invited lecture at the Pittsburgh Conference in Cleveland, OH, March 2.

Extended-chain Crystals. Lecture at the Carothers Laboratory of the DuPont Research Laboratory, Wilmington, DE, March 12.

DTA of Polymers. Lecture at the Film Department of the DuPont Research Laboratory, Wilmington, DE, March 13.

Polymerization of Polymer Crystals. Contributed lecture at the Am. Phys. Soc. Meeting in Dallas, TX, March 23–26.

Crystals of Linear Macromolecules. A short course of 8 lectures given for the Am. Chem. Soc. in Newark, DE, March 30–31.

DTA of Polymers. A lecture given at the Research laboratories of the DuPont Company, Richmond, VA, April 1.

The Solid State of Linear Macromolecules. A lecture given at the Research Labs of Owens Illinois Company, Toledo, OH, April 28.

Thermal Analysis of Polymers. A lecture given at the University of Detroit, Detroit, MI, April 29.

Travel to Germany to give a plenary lecture and attend a discussion meeting.

Ordnungszustände und Umwandlungserscheinungen in festen Hochpolymeren. Plenary lecture, Bunsentagung, Heidelberg, Germany, May 7–10.

Thermal Analysis of Linear Macromolecules. Seminar at the University of Mainz, Mainz, Germany, May 12.

1970, cont. DTA von Polymeren. Lecture at the Research Labs, BASF, Ludwigshafen, Germany, May 13.

Crystallization of Linear Macromolecules. Contribution to the first Gomadinger Discussion Meeting, Gomadingen, Germany, May 17–20.

Annealing and Crystal Growth in Polymers. Lecture in a Program on Materials Science at the University of Utah, Salt Lake City, UT, May 22.

Extended Chain Crystals. Lecture at Celanese Corporation, Summit, NJ, June 8.

Crystallization during Polymerization. Lecture at the Biennial Symposium of the Am. Chem. Soc. Polymer Division in Akron, OH, June 17.

[1970/71 Special Leave, remaining at RPI. Twelve months of a fully supported release from formal classroom assignments, but with fully maintained, externally supported, research activities was arranged instead of a formal sabbatic leave. This was to enable a number of activities supporting teaching: A.) The development of a new Freshman Chemistry Lecture Series (ultimately used in form of publ. 255, Appendix A) and, even more important, B.) The writing of a new book: "The Crystalline State of Linear High Polymers" (later renamed "Macromolecular Physics"), Volume 1, publ. 95a,b). (For the arrangement of this leave see the pages 8-57 and 67.)

The writing and final publication of the five sections of "Macromolecular Physics" is described for Volume 1, on page 8-58, and for Volumes 2 and 3 on page 8-62. The much later completed Volumes 4 and 5 were published under different titles, as mentioned on page 8-63.

No change in residence, 211 Winter St. Ext. Troy, NY.

1970, cont. (A) Thermoanalysis of Linear Macromolecules. (B) Extended Chain Crystals. (C) Helical Chain Conformation. Lectures and discussions at the Boeing Research Center, Seattle, WA, August 10–15.

Special trip to Europe to attend the IUPAC Symposium in Leiden, The Netherlands.

Defect Crystals. Discussion at the Research Laboratory of Union Carbide, Brussels, Belgium, August 25. (Dr. Ruland)

Melting of Crystals. Discussions at the University of Mainz, Mainz, Germany, August 26.

Thermodynamics of the Solid Polymers. Discussion at the BASF Research labs, Ludwigshafen, Germany, August 27.

Polymerization during Annealing of Poly(ethylene terephthalate). Lecture at the IUPAC Symposium on Macromolecules, Leiden, Netherlands, August 30–September 5.

Defect Crystals of Linear Macromolecules. Second Gomadinger Discussion Meeting, Gomadingen, Germany, September 7–9.

Crystallization of Poly(ethylene terephthalate). Lecture at the Farbwerke Höchst, Frankfurt-Höchst, Germany, September 10.

1970, cont. Strain Effects in Polymers. Lecture at the Research Laboratories, Owens-Illinois, Toledo, OH, September 24.

Orientation Effects in Polymers. Lecture at the Research Laboratories, Owens-Illinois, Toledo, OH, October 22.

Melting and Crystallization of Linear High Polymers under Pressure. Invited lecture at the NSF sponsored meeting on Pressure Effects in Polymers, MIT, Cambridge, MA, October 26–28.

Calorimetry of Polymers. Lecture at the Tennessee Eastman Research Laboratories in Kingsport, TN, November 5.

Research in Polymers. Discussion and visitation at Armstrong Cork Company, Lancaster, PA, December 15–17.

Thermal Analysis of Polymer Properties. Lecture at the Molecular Design and Application of Polymeric Materials Short Course Series, (Program Design) Cherry Hill, NJ, February 18.

1971 Annealing during Polymerization. Lecture at the Textile Fibers Department, DuPont Company, Waynesboro, VA, January 12.

Annealing of Poly(ethylene terephthalate). Lecture at the Plastics Department, DuPont Company, Wilmington, DE, January 20.

Nucleation in Polymers. Lecture at the Gordon Conference, Santa Barbara, CA, January 25–29.

Crystal Structure and Crystallization. Lecture at California Institute of Technology, Pasadena, CA, January 29 (followed by a trip to Mexico, see pages 8-93–95).

Thermal Analysis of Polymers. Lecture at the Plastics Department, DuPont Company, Wilmington, DE, February 16.

Crystallization and Polymerization. Lecture at the Chemistry Seminar Series, Rensselaer Polytechnic Institute Troy, NY, February 25.

(A) Time Dependent Heat Capacity in the Glass Transition Region. (B) M. Coughlin, Crystallization, Chain Folding and Chain Extension of Selenium. (C) A. Miyagi, Reversible Etching of Poly(ethylene terephthalate) Crystals. (D) S. Kubo, Crystallization During Polymerization of Poly-*p*-xylylene. Four contributed lectures at the Am. Phys. Soc. Meeting, Cleveland, Ohio, March 29–31.

(A) Crystal Structure and Crystallization. (B) Morphology and Melting. Two lectures at the Phillips Research Laboratories, Bartlesville, OK, April 2l–23.

Annealing of Poly(ethylene terephthalate). Lecture at the North Jersey Section of the American Chemical Society, South Orange, NJ, April 26.

Big Molecules. Lecture at Rensselaer Polytechnic Institute's Parents Weekend, Troy, NY, May 8.

Thermal Analysis. Lecture at the Research Laboratory, IBM, Endicott, NY, June 7.

Third ICTA in Switzerland (Mettler Award, see page 8-57.) *Later in the trip, I was joined by the family* (For a picture in Prague, see page 8-76.)

Polymer Science. A general discussion at the Technische Hochschule, Karlsruhe, Germany, August 17 (arranged by Professor Dr. B. Vollmert).

1971, cont. The Solid State of Linear Macromolecules. (A) Discussions at the Research Labs of the BASF, Ludwigshafen, Germany, August 18, and (B) Lecture at the University of Mainz, Mainz, Germany, August 19.

Taking Temperature and Pulse of Large Molecules. Mettler Award Address at the Third International Conference on Thermal Analysis, Davos, Switzerland, August 22–27.

(A) Fast Differential Thermal Analysis. (B) Differential Scanning Calorimetry at 150 atm Pressure. Two contributed papers at the Third International Conference on Thermal Analysis, Davos, Switzerland, August 22–27.

Extended Chain Crystals of Linear High Polymers. Main lecture at the 8th IUPAC Microsymposium on Macromolecules, Prague, Czechoslovakia, August 29–September 3.

End of the Special Leave.]

1971, Cont. Crystals and Crystallization of Polymers. Seminar at the University of Syracuse, Syracuse, NY, November 12.

Extended Chain Crystals. Lecture at the Owens-Illinois Research Center, Toledo, OH, November 30.

Crystallization and Melting of Macromolecules. Seminar at Rochester Institute of Technology, Rochester, NY, December 2.

Thermal Properties of Polymers. Lecture at the Research Laboratory, Xerox Company, Rochester, NY, December 3.

1972 Melting Point Variations in Polymers. Plenary lecture at the Third North American Thermal Analysis Society Meeting, Waco, TX, February 7–8.

Analysis by Calorimetry. Lecture at the Pittsburgh Conference on Analytical Chemistry, Cleveland, OH, March 7.

Etching of Polymers. Invited lecture at the Fibers Department, DuPont Company, Waynesboro, VA, March 29.

Morphology of Polymer Crystals. Lecture presented at Princeton University, Princeton, NJ, April 24.

Nucleation and Crystallization of Polymers. Lecture at the 4th Central Meeting of the Am. Chem. Soc., Pittsburgh, PA, May 4.

Trip to Poland (With Heidel June/July 1972, see pages 8-59–62.)

Crystallization of Linear Macromolecules With and Without Chain Folding. Invited lectures at (A) the Chemische Werke Hüls, Marl, June 6; (B) the BASF, Ludwigshafen, June 7; (C) the University of Mainz, Mainz, June 8; (D) Farbwerke Höchst, June 9; (E) the Bayer Laboratory, Dormagen, June 13; (F) the University of Marburg, Marburg, June 19; (G) the Faserforschungsinstitut, Teltow, June 22; (H) the Bundesanstalt für Materialprüfung, Berlin, June 23; (I) the National Academy of Science of Poland at the Technical University in Łódź, Poland, June 27; (J) the National Academy of Science of Poland at the Polymer Institute, Warszawa, Poland, June 28; and (K) the University of Ulm, Ulm, Germany, July 5.

1972, cont. Crystallization of Macromolecules. Lecture at the Research Laboratory of the Union Carbide Corporation, Tarrytown, NY, July 18.

Structural Data on Crystalline Polymers by Thermal Analysis. Lecture at Batelle Inst., Int. Symp. on Polymer Characterization, Seattle, WA, August 20–24.

The Place of Macromolecules in Freshman Chemistry. Invited plenary lecture at the Symp. Am. Chem. Soc. on Teaching Chemistry Through Macromolecules, New York, NY, August 28–29.

Crystallization and Chain Folding. Seminar at Case-Western Reserve University, Cleveland, OH, September 8.

1973 Transitions and Crystallization of Macromolecules. Two lectures at the U.S. Air Force Materials Laboratory, Dayton, OH, January 9.

Molecular Nucleation. Lecture at the Research Laboratory of the DuPont Co. Wilmington, DE, March 12.

Macromolecules and Teaching of Freshmen Chemistry. Lecture and discussion at the State University of North Carolina, Raleigh, NC, March 13.

Crystallization of Polymers from the Gaseous Monomer. Paper presented at the Am. Phys. Soc. Meeting, San Diego, CA, March 15–19.

(A) Etching and Annealing of Poly(ethylene terephthalate). (B) Crystallization of Polymers from the Gaseous Monomer. Two lectures at the Research Laboratories, IBM, San José, CA, March 22.

Tour Speaker for the Am. Chem. Soc., Prairie Circuit

How to Grow Large Crystals of Macromolecules. (A) Tulsa, OK, April 23; (B) Bartlesville, OK, April 24; and (C) Oklahoma City, OK, April 25.

Audio Courses on Thermal Analysis. Lecture at the Third Annual Meeting of the North American Thermal Analysis Society, Worcester, MA, June 11–14.

Molecular Nucleation. Invited Lecture to the Summer School Program, University of Utah, Salt Lake City, UT, July 16–17.

Chemical Reactions Involving the Backbone Chain of Macromolecular Crystals. Lecture at the NATO Conference on Reactions on Polymers at Rensselaer Polytechnic Institute, Troy, NY, July 23–26.

Chemistry and Physics of Large Molecules. Lecture at NSF Summer Program for Students organized at Rensselaer Polytechnic Institute, Troy, NY, August 3.

[1973/74 Second Sabbatic, remaining at RPI. Twelve months sabbatic with fully maintained, externally supported research activities. Given for the completion of Volume 2 of "Macromolecular Physics," publs. 102a,b of Appendix A and extended foreign travel (see pages 8-62 and 63).

No change in residence, 211 Winter St. Ext. Troy, NY. (See page C-5.)

1973, cont. *Trip Aberdeen, Scotland to the IUPAC Meeting and to teach in a Summer School for Calorimetry in Lyons, France*

Molecular Nucleation. Contribution to the IUPAC Meeting in Aberdeen, Scotland, September 10–14.

1973, cont. Crystallization of Macromolecules under Elevated Pressure. Lecture at the University of Bristol, Bristol, England, September 16–19.

Thermal Analysis of Linear Macromolecules. Lecture at the British Physical Society Meeting in Shrivenham, England, September 19–21

Thermal Analysis of Linear Macromolecules. Lecture at the Summer School on Thermal Analysis at the University of Lyons, Lyons, France, September 24–28. This was the only time, I experienced simultaneous translation of my lecture into French. (It took a major effort before the lecture to instruct the interpreter in the scientific terms likely to come up).

Polymerization during Crystallization. Lecture at the Polymer Institute, University of Grenoble, Grenoble, France, September, 29–30

Polymerization during Crystallization. Lecture and discussion at the Research Laboratories, DuPont Company, Wilmington, DE, October 8.

Crystallization of Macromolecules. Lecture at the Research Laboratories, DuPont Company, Kinston, NC, October 10.

Polymerization and Crystallization of Polyparaxylylene. Lecture at the Research Laboratory, Xerox, Rochester, NY, October 16.

Nucleation and Crystallization of Macromolecules. Lecture at the Research Laboratories, Ford Motor Company, Dearborn, MI, December 4 and at the General Electric Company, Schenectady, NY, December 10.

1974 Effect of Pressure on the Glass Transition of Macromolecules. Lecture at the Research Laboratories, DuPont Company, Wilmington, DE, February 11.

How to Make Large Crystals of Large Molecules. Lecture at the Susquehanna Valley Section, Am. Chem. Soc., Bloomsburg, PA, February 13.

Molecular Nucleation. Seminar at Case Western Reserve University, Cleveland, OH, March 1.

(A) Molecular Nucleation and Crystallization of Macromolecules. (B) G. Czornyj, Superheating during Melting of Extended Chain and Stirrer-crystallized Polyethylene. (C) A. Mehta, Segregation of Macromolecules on Crystallization. (D) M. Mucha, Morphology of Polyethylene Crystallized during Polymerization of Diazomethane. (E) R. C. Bopp, Crystallization during Polymerization of Polyparaxylylene. III. Thermal Analysis of Various Crystal Morphologies. Five contributed papers at the Am. Phys. Soc. Meeting, Philadelphia, PA, March 25–27.

Polymerization during Crystallization. Lecture at the Research Laboratories, Allied Chemical Company, Morristown, NJ, March 29.

Large Molecules. Lecture at Rensselaer Polytechnic Institute for Freshmen Chemists, Troy, NY, April 29.

(A) Transitions of Macromolecules. (B) Morphology of Macromolecular Crystals. Two lectures at the Summer School Program, State University of New York, New Paltz, NY, May 15.

Travel to Hungary to the Fourth, ICTA, with family, meeting with Hans and Inge in Budapest. Caryn continued her travel independently from Vienna to St. Moritz, Switzerland, to work at 'Randolins,' a hostel; (until August 30, see page 8-79).

1974, cont. Molecular Nucleation. Lecture at (A) the Research Laboratory, Bayer Chemical Company, Dormagen, Germany, June 18, and (B) the Research Laboratory of the BASF in Ludwigshafen, Germany, June 19.

Effect of Pressure on the Glass Transition of Linear Macromolecules. Lectures at (A) the University of Mainz, Mainz, Germany, June 24, and (B) the Farbwerke Höchst, Frankfurt-Höchst, Germany, June 25.

Heat Capacity of Linear Macromolecules. Invited lecture at the Fourth International Conference on Thermal Analysis (ICTA), Budapest, Hungary, July 7–13.

High Pressure DTA. Contributed paper at the Fourth International Conference on Thermal Analysis, Budapest, Hungary, July 7–13.

Charter Flight to the IUPAC Meeting in Brasil and stopover in Brasilia and Peru (For details see pages 8-32–35.)

Crystallization during Polymerization from the Gaseous and Liquid Monomer. A Lecture at the IUPAC Symposium on Macromolecular Chemistry, Rio de Janeiro, Brazil, July 26–31.

Crystallization during Polymerization from the Gaseous and Liquid Monomer. Lecture, Midland Macromolecular Meeting, Midland, MI, August 19–21.

End of the Second Sabbatic.]

1974, cont. Observation of New Trends in Polymer Science. Lecture at the Research Laboratory, Plastics Department, DuPont Company, Wilmington, DE, October 16.

Tour Speaker on the Lake Erie Circuit, American Chemical Society

The Solid State of Large Molecules. Lecture at the Penn-York Section, Fredonia, NY, November 5.

Modern Chemistry. Lecture at the State University College in Fredonia, NY, November 5.

The Solid State of Large Molecules. Lecture at the Erie Section of the American Chemical Society, Erie, PA, November 6.

Modern Chemistry. Lecture at Mercyhurst College, Erie, PA, November 6.

The Solid State of Large Molecules. Lecture at the Northeastern Ohio Section in Painesville, OH, November 7.

Modern Chemistry. Lecture at the Penn-Ohio Border Section in Warren, OH, November 8.

Crystallization during Polymerization. Lecture at the Research Laboratories, DuPont Company, Kinston, SC, November 18.

1975 Vibrational and Rotational Contributions to the Heat Capacity of Linear Macromolecules. Lecture at the Massachusetts Institute of Technology, Boston, MA, January 6.

Time Dependent Differential Thermal Analysis. Lecture at the Experimental Station, DuPont Company, Wilmington, DE, January 28.

Morphology of Polymer Crystals. Lecture at the State University of New York, Albany, NY, March 11.

(A) Orbital Control of Crystallization during Polymerization. (B) R. C. Bopp, Thermal Analysis of Paraxylylene Polymers and Oligomers. (C) Polymer Heat Capacities. (D) Molecular Physics Taught via Audio Courses. Four contributed papers at the American Physical Society Meeting, Denver, CO, March 31–April 3.

(A) Polymer Crystal Nucleation and Growth from the Monomer. (B) Molecular Weight Separation on Crystallization. (C) C. J. Lee, Crystallization During Polymerization of Divalent Compounds Through Chemical Transport Reaction. Three invited lectures at the American Chemical Society Meeting in Philadelphia, PA, April 7–8.

Copolymer Effects on Melting and Glass Transition. Lecture at the Experimental Station, DuPont, Wilmington, DE, April 16.

Morphology of Polymer Crystals. Lecture at the State University of New York, Binghamton, NY, April 2.

Chemistry of Small and Large Molecules. Lecture at the 37th Summer Conference of the New England Association of Chemistry Teachers, Williamstown, MA, August 12.

(A) Melting and Crystallization of Linear Macromolecules. (B) Heats of Transition by Calculator Connected DSC. Two invited lectures at the American Chemical Society Meeting, Chicago, IL, August 25–29.

Crystals of Linear Macromolecules. Lecture at the Capital District Research Directors Meeting, Albany, NY, October 1.

Annealing and Sintering of Linear Macromolecules. Lecture at the Plastics Department, Research Laboratories, DuPont Company, Wilmington, DE, October 7.

The Solid State of Linear Macromolecules. Lecture at the Local ACS Section in Buffalo, NY, October 29.

Molecular Nucleation. Lecture, University of Buffalo, Buffalo, NY, October 30.

Audio Course on Thermal Analysis of Linear Macromolecules. Lectures given at the Ethicon Co., with discussions to support the Audio Course taken by a group of the employees, Somerville, NJ, November 6 and November 20.

(A) Graduate Education in Polymer Science. (B) Melting and Crystallization of Linear Macromolecules. Two Lectures at the North American Chemical Conference, Mexico City, Mexico, December 1–5 (accompanied by Heidel).

1976 Nucleation, Crystallization, and Annealing. Invited contribution at the Gordon Conference on Polymers, Santa Barbara, CA, January, 12–13.

Taking the Temperatures and Pulse of Linear Macromolecules. North Jersey Am. Chem. Soc., Local Section Meeting, Orange, NJ, January 26.

Tour Speaker for the Am. Chem. Soc., Lakes Land Circuit

1976, cont. Chemical and Physical Nucleation of Linear Macromolecules. Am. Chem. Soc., Local Section Meeting, Midland, MI, February 3.

Audio Courses, Do they Eliminate the Need for Professors and Universities. Am. Chem. Soc., Local Section Meeting, Flint, MI, February 4.

Chemical and Physical Nucleation of Linear Macromolecules. Am. Chem. Soc., Local Section Meeting, (A) Toledo, OH, February 5 and (B) Local Section Meeting, Fort Wayne, IN, February 6.

Molecular Nucleation. Lectures at (A) Lehigh University, Bethlehem, PA, February, 12 and (B) U.S. Bureau of Standards, Washington, D.C., March 22.

Crystallization of Linear Macromolecules. Seminar at Richmond College, Graduate Center, New York, NY, May 6.

Travel to Europe, Moretonhampstead Conference (Afterwards joined by Heidel.)

Molecular Nucleation. Plenary Lecture at the 16th Conference of the British High Polymer Research Group, Moretonhampstead, England, May 11–13.

High Pressure Crystallization. (A) Seminar at the University of Reading, Reading, May 14 and (B) at the National Physics Laboratory, Teddington, May 15. (Dr. M. Richardson). Then traveled to continental Europe to meet Heidel.

Das Polymerisieren von Diphenylsiliziumkristallen. Lecture at (A) the University of Mainz, May 20 and (B) the Research Laboratory, Farbwerke Höchst, May 21, followed by a vacation in the Glottertal and continued travel.

Molecular Nucleation. Colloquium at the National Research Laboratory, Strasbourg, France, June 1.

(A) Das Polymerisieren von Diphenylsiliziumkristallen. (B) Molecular Nucleation. Two lectures at the Research Laboratory, BASF, Ludwigshafen, Germany, June 2.

Molecular Nucleation. Lecture, University of Marburg, Marburg, Germany, June 3.

Crystallization and Melting of Linear Macromolecules. Lecture and chairing of panel discussions, IUPAC Microsymposium, Brussels, Belgium, June 8.

New Directions of Polymer Research in Europe. Lecture at the Experimental Station, DuPont Company, Wilmington, DE, June 15.

Crystallization of Linear Macromolecules. Invited lecture and discussion at the Gordon Research Conference on Crystal Growth, Andover, NH, July 12–17.

Crystallization and Melting of Linear Macromolecules. Lecture at the IBM Research Lab, Yorktown Heights, NY, August 25.

1977 Equilibrium Melting of Linear Macromolecules. Lecture at the Thermal Analysis Group, DuPont Research Lab, Wilmington, DE, February 10.

Crystallization during Polymerization. Lecture at the American Physical Society Meeting, San Diego, March 21–24.

How to Crystallize Large Molecules. Lecture at the Local ACS Meeting in Wilmington, DE, April 19.

1977, cont. Crystallization During Polymerization from the Gas Phase. Lecture at the Canadian Institute of Chemistry (CIC) and ACS Symposium, Montreal, May 30.

How to Grow Large Crystals of Linear Macromolecules. Plenary lecture at the Fifth International Crystal Growers Conference (ICCG5), Boston, MA, July 18–22.

Lectures and discussions in Venezuela based on Audio Courses (see page 8-68)
At the IVIC, the Instituto Venezolano de Investigaciones Cientificas, in Caracas
Research in Polymer Science and Thermal Analysis. Discussion series of 6 lectures at IVIC, Caracas, Venezuela, August 1–4. (Dr. Antonio Muñoz-Escalona).

Equilibrium Melting of Macromolecules. Invited lecture, Am. Chem. Soc. Meeting, Chicago, IL, September 1.

How to Grow Large Crystals of Linear Macromolecules. Invited lecture at the Akron Lecture Group, Akron, OH, October 7.

How to Take the Pulse and Temperature of a Linear Macromolecule. Lecture at the American Cyanamid Co., Stamford, CN, October 25.

Heat Capacities of Linear Macromolecules. Lecture at the North Jersey ACS Section, Newark, NJ, October 31.

Equilibrium Crystals of Linear Macromolecules. Lecture at Allied Chemical Co., Morristown, NJ, November 1.

Chain Extension of Linear Macromolecules. Lecture at the Pioneering Research Dept, Textile Fibers Div., DuPont Co., Wilmington, DE, November 15.

1978 Chain Extension of Linear Macromolecules. Lecture at the Celanese Research Laboratories, Summit, NJ, January 17.

(A) Crystallization During Polymerization of LiH_2PO4. Lecture at the Am. Phys. Soc. Meeting, and (B) U. Gaur, Addition Scheme for Heat Capacities of Linear Macromolecules. Poster, Washington, DC, March 27–30.

A New System of Subdividing of Chemistry. Lecture at the Hudson Local ACS Section, Newburgh, NY, April 25.

Thermal Analysis of Amorphous Macromolecules. Lecture given at the Elastomers Dept., DuPont Co., Wilmington, DE, June 13.

Second set of lectures and discussions in Venezuela (With Heidel, stop in Curacao.)
At the Instituto Venezolano de Investigaciones Cientificas in Caracas (see page 8-68)
How to Grow Extended Chain Crystals of Linear Macromolecules. Lecture at IVIC, Caracas, Venezuela, August 25. (Dr. Antonio Muñoz-Escalona).
Crystals of Linear Macromolecules. A series of 16 lectures and 8 laboratory sessions at the IVIC, Caracas, Venezuela, August 21–September 1.

Crystallization and Melting of Linear Macromolecules. Lecture at the Dept. of Chemistry, Univ. of Virginia, Charlottesville, VA, October 2.

1978, cont. The Glass Transition in Macromolecules. Seminar at the Marshal Lab, DuPont Co., Philadelphia, October 23.

Thermal Analysis of Amorphous Polymers. Lecture and discussion given for the Society of Plastics Engineers Meeting, Chicago, IL, November 15.

1979 Thermal Analysis of Copolymers. Lecture at the Thermal Analysis Club of the DuPont Co., Wilmington, DE, February 8.

Thermal Analysis of Amorphous Polymers. Lecture and discussions for the Soc. of Plastics Engineers Meetings, Cleveland, OH, March 6.

Tour Speaker for the Am. Chem. Soc., New York Circuit

Should We Update Teaching of Chemistry. Lecture at ACS Local Section at Potsdam, NY, March 15.

A New System to Describe all Types of Matter. Lecture at the ACS Local Section at Corning, NY, March 20.

Should We Update Teaching of Chemistry. Lecture at the ACS Local Section at Norwich, NY, March 21.

A New System to Describe all Types of Matter. Lecture at the ACS Local Section in Syracuse, NY, March 22.

Crystallization of Se and Lithium Phosphate. Lecture presented at the Research Laboratories of the Ethicon Co., Somerville, NJ, April 23.

Thermal Analysis of Crystalline Copolymers. (A) Lecture at the ACS Local Section in Newark, NJ, April 23 and (B) lecture and discussion given for the Society of Plastics Engineers Meeting, New Orleans, LA, May 8.

Thermal Characterization of Materials. Lecture and discussion at the Polytechnic Institute of New York, NY, May 15.

Thermal Analysis and Structure of Semicrystalline Macromolecules. Tutorial lecture and discussion at the Delaware ACS Section, Wilmington, DE, June 6.

Crystallization of Linear Macromolecules. Lecture at the Plastics Dept. of the DuPont Co., Wilmington, DE, June 7.

Trip to Europe for a Plenary Lecture at the IUPAC (With Heidel, see page 9-33.)

Modern Application of Thermal Analysis. An invited lecture at the E. Kuhlman Co., Paris, France, July 4.

Spezifische Wärmen von Linearen Hochpolymeren. Lecture at the Univ. of Freiburg, Germany, July 6.

Se and $LiPO_3$ als Modellverbindungen linearer Hochpolymerer. Lecture at (A) the BASF, Ludwigshafen, Germany, July 9; (B) the University of Mainz, Germany, July 10; (C) the Farbwerke Höchst, Frankfurt-Höchst, Germany, July 11; and (D) the University of Ulm, Germany, July 13.

Specific Heats of Linear Macromolecules. Plenary Lecture at the IUPAC Symposium on Thermal Analysis, Prague, Czechoslovakia, July 16–20.

(A) Additivity of the Heat Capacity of Linear Macromolecules in the Solid State. Contributed lecture and (B) Graduate Instruction in Macromolecular Science

through Audio Courses. Invited lectures, given at the Am. Chem. Soc. Meeting in Washington, DC, September 10–13.

Travel to Englnd, to contribute an invited lecture to the 1st International Meeting on Polymer Crystallization in Cambridge, England, September 25–28 (See page 8-63.) Molecular Nucleation and Segregation, given at the Faraday Society Discussions of the Chemical Society (Discussion No. 68, held under the title: 'Organization of Macromolecules in the Condensed Phase.' (See Appendix A #160.)

1979, cont. Thermal Analysis of Linear Macromolecules. Lecture at the Research Laboratory of Stauffer Chemicals, Dobbs Ferry, NY, November 13.

LiPO3 and Se as Model Compounds of Linear Macromolecules. Seminar at the Univ. of Massachusetts, Amherst, MA, November 16.

1980 *NSF supported travel to the International Symposium on 'New Frontiers in Polymer Science and Polymer Applications' in Madras, India* (See pages 8-95–96.)
(This included a ½ h nationally televised round-table discussion with Professor Bamford, the IUPAC representative, and Dr. Ramanathan, the organizer.)

Irreversible Melting of Linear Macromolecules. Plenary lecture at the Symposium in Madras, India, January 7–10.

$LiPO_3$ and Se as Model Compounds of Linear Macromolecules. Seminar at the Indian Institute of Technology, Madras, India, January 10.

Melting of Linear Macromolecules. Discussion at the Leather Institute of Madras, India, January 11.

Irreversible Melting. Seminar at the University of Delhi, India, January 14.

Thermal Analysis. Lecture at the Thermal Analysis Forum of the DuPont Company in Wilmington, Delaware, February 14.

(A) The Glass Transition in Polyethylene. (B) U. Gaur, Polymer Heat Capacity Data Bank (Poster). (C) Glass Transition of Mesophase Macromolecules. (D) K. Fisher, Changes in the Crystalline Content of PTFE induced by Radiation (Poster) at the Am. Phys. Soc. Meeting in New York, NY, March 24–27.

Melting of Macromolecules. Lecture, Polytechnic Institute of New York, April 16.

Phase Transitions in Linear Macromolecules. Lectures at (A) the University of Michigan, Ann Arbor, April 28 and (B) the Midland Molecular Institute, Midland, Michigan, April 29.

The Basis of Thermal Analysis. Lecture for a Short Course on Thermal Analysis at the Polytechnic Institute of New York, NY, May 13.

Thermal Analysis of Amorphous Polymers. Lecture at the SPE Symposium in the Poconos, New Jersey, May 21.

Melting of Crystalline Macromolecules Important to Polymer Industry. Lecture at the DuPont Laboratories, Seaford Plant, Seaford, Delaware, June 2.

1980, cont. Glass Transitions of Linear Macromolecules. An invited lecture at the International Symposium on Phase Transitions, held at the Case Western Reserve University, Cleveland, Ohio, June 11.

Travel to the 6th ICTA in Bayreuth, Germany (Accompanied by Heidel.)

1980, cont. Spezifische Wärme im Glasumwandlungsbereich. Lecture at (A) the Kunststoff-Seminar, T.U. and (B) B.A.M. Berlin, Germany, July 3.

Addition Scheme for Heat Capacities of Linear Macromolecules. Paper given at the 6th ICTA in Bayreuth, Germany, July 6–12.

Neue Experimente über die Glasumwandlung. Lectures given at (A) the T.U. in Clausthal, Germany, July 14 and (B) the Research Laboratories of the Bayer AG in Dormagen, Germany, July 16.

The Glass Transition of Macromolecules. Colloquium at the University of Leuven, Belgium, July 17.

[1980/81 Third Sabbatic, remaining in Troy. Fully supported, for one semester, with externally supported research activities maintained (see also page 8-86). It was to: 1.) Produce an audio course on thermal analysis (see Appendix A #184); 2.) Develop a proposal for a thermal analysis laboratory course. (Report submitted, funds for equipment raised, and the instrumentation installed into our thermal analysis research laboratory, ATHAS. It was made available to undergraduate and graduate students under supervision of operators from our laboratory.)

No change in residence, 211 Winter St. Ext. Troy, NY. (See page C-5.)

1980, cont. The Basis of Thermal Analysis. Seminar for the DuPont Instrument Division, held in Albany, NY on October 3.

Phase Transitions of Linear Macromolecules. Lecture at the Allied Corporate Research Center, Morristown, NJ, November 18.

(A) Determination of the History of a Solid by Thermal Analysis. Invited lecture, and (B) P. H.-C. Shu, Thermal Properties of Selenium. Lecture at the Eastern Analytical Symposium in New York City, NY, November 19.

Design of Differential Scanning Calorimetry Instruments. Lecture at the DuPont Instrument Division, Wilmington, DE, December 1.

1981 Transitions in Mesophase Polymers. Lecture at the PPD Department of the DuPont Company, Wilmington, DE, January 21.

ATHAS News on Glass Transitions. Lecture for the Thermal Analysis Group, Experimental Station, DuPont Company, Wilmington, DE, January 22

Transitions in Mesophase Polymers. A seminar at the University of Lowell, Lowell, MA, January 28.

End of the Third Sabbatic.]

1981, cont. History of Materials Analyzed by Thermal Means. Lecture at the Union Carbide Research Labs, Bound Brook, NJ, February 16.

Structural, Thermodynamic and Mechanical Properties of Polymers, (A) Introduction, (B) The Solid State, and (C) Solid-Liquid Transitions. Three lectures given at an APS Short Course, Phoenix, Arizona, March 14–15.

(A) The Role of the ATHAS Heat Capacity Data Bank in Recent Advances in the Understanding of the Glass Transition. (B) R. Bopp, Glass Transition Behavior of Brominated Copolymers of Poly(2,6-dimethyl-1,4-phenylene oxide). (C) ATHAS Data Bank of Macromolecular Heat Capacities (Poster). Presentations at the APS March Meeting, Phoenix, Arizona, March 18.

History of Polymers by Thermal Analysis. Lecture at the G.E. Silicone Research Facility, Waterford, NY, March 23.

Differential Scanning Calorimetry as a Tool in Polymer Analysis. Invited lecture at the ACS Meeting in Atlanta, GA, April 2.

Crystals of Linear Macromolecules. Lecture at the University of Detroit, Detroit MI, May 19.

The Basis of Thermal Analysis. A lecture in a Short Course on Thermal Analysis at the Polytechnic Institute of New York, NY, May 12.

U. Gaur, The ATHAS Polymer Heat Capacity Data Bank. Presentation at the ACS Meeting, New York, NY, August 27.

The Glass Transition in Polymers. Lecture at a seminar at the General Foods Company, Research Center in Terrytown, NY, September 22.

Nucleation and Crystallization of Linear Macromolecules. Lecture at the Research Laboraratories of the DuPont Co. in Parkersburg, Virginia, October 2.

Thermal Analysis of Linear Macromolecules. Lecture at the State University of New York, Albany, NY, October 9.

The Impact of Computers on Thermal Analysis. A special, distinguished invited lecture, given at the Eastern Analytical Symposium of the ACS in New York, NY, November 19.

The Need for a Thermal Analysis Center. Invited lecture at the DuPont Instrument Company, Wilmington, DE, December 18.

1982 Transitions in Linear Macromolecules. Lecture at the Hercules Research Center in Wilmington, DE, January, 12.

Travel to give the Plenary Lecture at the German Physical Society Meeting

(A) Ist die Polymerphysik unterentwickelt? Plenary lecture (see also page 7-20), and (B) Berechnung der Wärmekapazität aus dem Schwingungsspektrum und Ermittlung der Thetatemperaturen aus der Wärmekapazität. The second lecture was a contributed lecture. Both were given at the German Physical Society Meeting in Regensburg, March 14–17.

Die Glasumwandlung in Mesophasen. Lecture at the University of Marburg, Germany, March 18.

Die Glasumwandlung in Linearen Hochpolymeren. Lecture at the Research Laboratories Farbwerke Höchst, Frankfurt-Höchst, Germany, March 19.

1982, cont. Die Glasumwandlung in Mesophasen. Lectures at (A) the University of Mainz, Germany, March 22, (B) the BASF, Ludwigshafen, Germany, March 23, (C) the University of Freiburg, Germany, March 24, and (D) Bayer in Leverkusen, Germany, March 25.

Mesophases of linear Macromolecules. Sigma Xi Lecture at (A) the Uniroyal Chapter in Middlebury, CT, April 14 and (B) the Delaware Thermal Analysis Group in Wilmington, DE, April 15 (Round trip by automobile).

Thermal Analysis of Block Copolymers. Lecture at the DuPont Thermal Analysis Club in Wilmington, DE, April 15.

Mesophases of linear Macromolecules. Lecture in the Chemistry Dept. Seminar Series of Rensselaer Polytechnic Institute, Troy, NY, April 22.

Thermal Analysis of Mesophases. Invited lecture at Bailor University on the occasion of the 'Malcolm Dole Symposium,' Waco, TX, April 30–May 1.

The Role of Small Crystals in the Properties of Segmented Polyurethanes. Lecture at the Research Laboratory of the Textile Research Department of the DuPont Co. in Waynesboro, VA, May 4.

Thermal Analysis of Mesophases. Seminar at Virginia Polytechnic Institute, Blacksburg, VA, May 5.

The Characterization of Solid Linear Macromolecules. A two-day Short Course for EXXON in Linden, NJ, (4 two-hour lectures and discussion), May 17–18.

The Basis of Thermal Analysis. Lecture in a Short Course on Thermal Analysis at New York Institute of Technology, New York, NY, May 19.

ATHAS Heat Capacity Data Bank. Lecture at the IUPAC symposium at the University of Massachusetts, July 11–16.

The Importance of Mesophase Structures in Pitches. Lecture at the Ashland Petroleum Co., Ashland, KY August 3.

(A) The Glass Transition of Mesophase Macromolecules. (B) The ATHAS Data Bank of Heat Capacities of Linear Macromolecules. Lectures at the 7th ICTA Symposium at Queens University, Kingston, Ontario, Canada, August 22–28.

Mesophase Macromolecules. Lecture at SUNY, College of Forestry, Syracuse, NY, September 15.

Understanding Polymer Science. Lecture at the 1982 Fall Institute of SUNY at Lake Mohonk, New Paltz, NY, November 2–5.

1983 How to Grow Large Crystals of Linear Macromolecules. Invited lecture at the Akron Lecture Group, Akron, OH, October 7.

Characterization of Macromolecules by Thermal Analysis. (B) Introduction to a Computer Assisted Audio Course on Thermal Analysis. Contributions to a Short Course at the Golden Gate Chapter of the Soc. of Plastics Eng., San José, CA, March 17.

Thermotropic Mesophase Polymers. Lecture at the IBM Research Laboratory in San José, CA, March 18.

A New Type of Mesophase for Macromolecules. Contributed Paper to the Am. Phys. Soc. Meeting in Los Angeles, CA, March 21–25.

1983, cont. Thermal Analysis of Isotactic Polypropylene. Invited Lecture at the 17th Middle Atlantic Regional Am. Chem. Soc., White Haven, PA, April 6–8.

Projection of an Advanced Thermal Analysis System. Lecture for the Thermal Analysis Group at the Experimental Station of the DuPont Company, in Wilmington, DE., April 11.

Thermotropic Mesophase Polymers. Lecture at the Bell Telephone Research Laboratory in Murray Hill, NJ, April 25.

Introduction to a Computer Assisted Audio Course on Thermal Analysis. Lecture at the North Jersey Section of the American Chemical Society at their local meeting in Newark, NJ, April, 25.

The Basis of Thermal Analysis. Lecture for a Short Course on Thermal Analysis at the Polytechnic Institute of New York, NY, May 11.

Travel on a Fellowship of the Japanese Society for the Promotion of Science
(Travel with Heidel, more details are given in Chapter 8, pages 8-97–99.)

Molecular Nucleation of Polymeric Crystals. Lecture at Kyoto University, Kyoto, Japan, May 19.

Thermotropic Mesophases. Lectures (A) at the Toyobo Co., Atata, Japan, May 20, (B) at the 32nd Japan Polymer Soc. Meeting in Kyoto, Japan, May 24, and (C) at Tokyo Metropolitan University, Tokyo, Japan, May 26.

Molecular Nucleation of Polymeric Crystals. Lecture at Tokyo University, of Agriculture and Technology, Tokyo, Japan, May 28.

Thermotropic Mesophases. Lecture at Hokkaido University in Sapporo, Hokkaido, Japan on May 31.

Molecular Nucleation of Polymeric Crystals. Lecture at Hokkaido University, Sapporo, Japan, June 1.

Heat Capacity of Linear Macromolecules. Lecture at Osaka University, Osaka, Japan, June 3.

Molecular Nucleation of Polymeric Crystals. Lectures at Okayama University, Okayama, Japan, June 4 and at Kuraray Co., Kurashiki, Japan, June 6.

Thermotropic Mesophases. Lecture at the Kuraray Co., Kurashiki, Japan, June 6.

Molecular Nucleation of Polymeric Crystals. Lectures at Hiroshima University, Hiroshima, Japan, June 7 and at the Mitsui Co., Iwakuni, Japan, June 8.

Thermotropic Mesophases. Lecture at the Mitsui Co., Iwakuni, Japan, June 9.

Heat Capacity of Linear Macromolecules. Lecture at Kyushu University, Fukuoka, Japan, June 10.

Molecular Nucleation of Polymeric Crystals. Lectures at (A) Tokyo University, Tokyo, Japan, June 13 and (B) the Research Institute for Polymers and Textiles, Tsukuba, Japan, June 14.

Teaching with the ATARI 800. Seminar at Rensselaer Polytechnic Institute, Troy, NY (Summer Course on Computers) June 24.

Do Condis Crystals Exist? Invited Lecture the ACS Meeting, Washington DC, August 28.

1983, cont. Thermal Analysis of Crystals, Glasses and Mesophases. Lecture at MMM in St. Paul MN, September 14.

DSC and DTA. Tutorial Lecture at the 12th North Am. Thermal Anal. Soc. in Williamsburg, VA, September 25–29.

(A) The Condis State of Small and Large Molecules. (B) H. G. Wiedemann, Investigation and Discussion of Liquid Crystals, Plastic Crystals, and Condis Crystals by Microscopy and Calorimetry. (C) S. F. Lau, The Condis State of Polytetrafluoroethylene. (D) J. Grebowicz, The Condis State of Polypropylene. Lectures at the 12th North Am. Thermal Anal. Soc. in Williamsburg, VA, September 25–29.

Travel to give the Plenary Lecture at the 10th Gefta Meeting in Germany

1984 Characterization of Macromolecules by Thermal Analysis. Discussion at the University of Paderborn, Paderborn, Germany, March 16.

Entwicklungstendenzen in der Thermoanalyse. Plenary Lecture at the 10th Gefta Meeting in Paderborn, Germany, March 19–21.

Thermal Analysis. Discussion at the Institute for Inorganic Chemistry of the University of Kassel, Germany, March 22.

(A) The Role of Condis Crystals in Crystallization of Macromolecules. (B) H. Suzuki, Calorimetric Study of Poly(oxymethylene). (C) J. Grebowicz, The A_o Parameter for Calculations of Heat Capacity of Polymers at Constant Pressure. (D) S. Z. D. Cheng, Molecular Nucleation of Polyethylene Oxide. (E). M.-Y. Cao, Addition Scheme for Heat Capacities of Linear Macromolecules. Five contributed papers to the Meeting of the American Physical Society in Detroit, MI, March 26–30.

Characterization of Conformationally Disordered Crystals by DSC. Invited lecture at the American Chemical Society Meeting in St. Louis, April 8–13.

New Results in Heat Capacities of Macromolecules. Lecture at the National Bureau of Standards Washington, DC, May 3.

The Basis of Thermal Analysis. Lecture in a short course on Thermal Analysis at the Polytechnic Institute of New York, NY, May 7–9.

First invited lecture series in China (Travel with Heidel from May 9 to June 7.) The lectures were translated by S. Z. D. Cheng; 500 slides were used. Train travel to Suzou (5/13), to Hangzhou (5/19–20), Hefei and Nanjing (5/25–31). Flight to Beijing and back to Shanghai (6/1 and 5). (Each lecture and discussion day also had a ½ day of sightseeing component, for more details see Chapter 8, pages 99–107).

1984, cont. (A) The Structure of Molecules and Phases. (B) The Glassy State. (C) Crystallization of Linear Macromolecules. (D) Crystals of Linear Macromolecules. (E) Morphology of Crystals of Linear Macromolecules. (F) The Melting Equilibrium of Linear Macromolecules. (G) The Irreversible Melting of Linear Macromolecules. (H) The Mesophases of Linear Macromolecules. (I) Copolymers and Blends of Linear

Macromolecules. (J) Heat Capacities of Linear Macromolecules. Ten lectures of 3 h each, equivalent to a full semester's material. East China Institute of Textile Science and Technology in Shanghai, China, May 12–23.

1984, cont. Linear Macromolecules. Discussion at the Jing-shan Chemical Complex Shanghai, China, and tour of the production facilities, (by bus) May 24.

(A) Mesophases of Linear Macromolecules. (B) Thermal Analysis of Copolymers and Blends and (C) a discussion on Research in Polymers. At the University of Science and Technology of China, Hefei, (travel by train) May 25–27.

Mesophases. Lecture at Nanjing Institute of Technology Nanjing, China, May 29.

Melting of Copolymers and Blends. Lecture at Nanjing Institute of Technology Nanjing, China, May 30.

Research in Polymers. Discussion at Nanjing Institute of Technology Nanjing, China, May 31.

Mesophases of Macromolecules. Lecture at the Beijing Institute of Technology Beijing, China, June 2.

(A) Melting and Thermal Analysis of Linear Macromolecules. (B) Heat Capacity of Linear Macromolecules. Two lectures at the Beijing Institute of Technology Beijing, China, June 4–5.

Discussion of cooperative research with Professor Qian and staff after return flight to Shanghai. At the East China Institute of Textile Sci. and Tech., June 6.

Condis Crystals. Invited Lecture at the first Gordon Conference on Liquid Crystals, New London, NH, July 8–14.

J. Grebowicz, Condis Crystals of Linear Macromolecules. Poster Presented at the first Gordon Conference on Liquid Crystals, New London, NH, July 8–14.

(A) The Measurement of High Precision Heat Capacity by DSC. (B) J. Menczel, The Glass Transition of Poly(ethylene terephthalate). Invited and contributed lectures at the 13th NATAS Meeting in Philadelphia, PA, September 23–26.

Travel to Europe, to give the Plenary Lecture at the Meeting of the Italian Association for Thermal Analysis and Calorimetry

The Glass and Melting Transitions of Polymers. Discussion at the University of Rome, Italy, December 3.

Precision Heat Capacity Measurements for the Characterization of Two-phase Polymers. Plenary Lecture at the Meeting of the Italian Association for Thermal Analysis and Calorimetry, Naples, Italy, December 4–7.

Condis Crystals of Linear Macromolecules. Lecture at the University of Naples, Naples, Italy, December 6.

1985 Transitions in Mesophases of Macromolecules. Invited Lecture at the Polymer Forum of the DuPont Co., Wilmington, DE, January 10.

The Physical Chemistry of Polyethylene. Invited Lecture at the Mobil Chemical Co., Edison, NJ, February 20.

1985, cont. The Use of Audiotape, Videotape, and Computers in Teaching of Specialized Graduate Courses. Seminar and Demonstration at the Physics Department of RPI, Troy, NY, February 22.

Tour Speaker for the American Chemical Society, Mid West Circuit

1985, cont. Thermal Analysis. (A) Wabash Valley Section, Terre Haute, IN, March 12, and (B) Louisville Section, Louisville, KY, March 14. (C) Thermotropic Mesophases. Indiana-Kentucky Border Section, Mt. Vernon, IN, March 13.

(A) Thermal Analysis of the Condis Crystals of Poly-*p*-xylylene. (B) S. Z. D. Cheng and The Kinetics of Molecular Nucleation. Two contributed lectures, and (C) M.-Y. Cao, Thermal Analysis of the Condis Crystals of Polydiethylsiloxane and Cyclosilanes. (D) J. Grebowicz, Thermal Analysis of the Condis Crystals of Poly-trans-butadiene. (E) K. Loufakis, Computation of Heat Capacities at Constant Volume and Pressure for Fluorinated and Brominated Polyethylene, three posters, presented at the American Physical Society Meeting in Baltimore, MD, March 25–39. (See page 8-107 and 108.)

Condis Crystals in Biological Polymers. Seminar for General Foods Visitation Group at RPI, Troy NY, April 10.

(A) Application of Differential Scanning Calorimetry to Polymers. Invited tutorial, and (B) Thermal Analysis of Liquid and Condis Crystals. Invited Plenary Lecture at the American Chemical Society Meeting, Miami Beach, Florida, April 28–May 3.

The Basis of Thermal Analysis. Lecture in a course on Thermal Analysis at the Polytechnic Institute of New York, NY, May 13–15.

Thermal Analysis in Materials Science. Invited Lecture at Oak Ridge National Laboratories, ORNL, Oak Ridge, TN, May 28. (See page 8-108.)

Basics and Future Developments of Thermal Analysis. Invited Lecture at the Gordon Conference on Analytical Pyrolysis at the Holderness School, Plymouth, NH, July 15.

Invitation to the ICTAC Workshop in Bratislava (Travel with Heidel.)

Qantitative Thermal Analysis of Macromolecular Glasses and Crystals. Plenary Lecture, 8th ICTA Symposium in Bratislava, Czechoslovakia, August 19–23.

The Use of Computers in Thermal Analysis. Invited Lecture and Workshop at the 8th ICTA Symposium in Bratislava, Czechoslovakia, August 19–23.

The Thermal Analysis of Glassy Macromolecules. Invited Lecture at the Prague Institute of Chemical Technology, Prague, Czechoslovakia, August 26.

Die Thermoanalyse von Gläsern. Invited Lecture at the Research Center of the BASF, Ludwigshafen, Germany, August 27.

Thermal Analysis. Invited, computer-illustrated lecture, New England Thermal Forum, Natick, MA, October 29.

1986 Thermal Analysis of Linear Macromolecules. Lecture at Penn State University, State College, PA, February 13.

(A) K. Loufakis, Conformational Analysis of Poly(vinylidene fluoride). Poster ; (B) S. Z. D. Cheng, Thermal Analysis of High-melting Polymers. (C) The Condis State of Small Molecules and two contributed lectures at the Am. Phys. Soc. Meeting in Las Vegas, NV, March 31–April 4.

(A) *W. Aycock, Heat Capacities of Rubber Polymers. Poster, April 10; (B) *K. Loufakis, Thermal Analysis of Poly(vinylidene fluoride). Invited lecture, April 15. Both at the Meeting of the Am. Chem. Soc. New York, NY.

Mesophases of Linear Macromolecules. Invited lecture at the University of Tennessee, Knoxville, TN, April 22. (See page 8-112.)

Glass Transitions of Copolymers. Seminar at the Delaware Thermal Analysis Forum, Wilmington, DE, April 28.

Thermal Analysis of Liquid Crystalline Polymers. Lecture at the Research Laboratories of Hercules, Inc., Wilmington, DE, April 29.

The Basis of Thermal Analysis. Lecture in a short course on Thermal Analysis at the Polytechnic Institute of New York, NY, May 13–15.

Glass Transition Analysis for Polymers of Interest for Optical Lenses. Invited Lecture at the Sola Syntex Co. in Phoenix, AZ, June 11.

S. Z. D. Cheng, Thermal Analysis of Mesophases. Invited Poster at the Gordon Conference on Liquid Crystals, New London, NH, July 8–11.

Thermal Analysis of Phase Transitions. Lecture at Pfizer, Groton, CT, September 5.

Detection of Phase Separation of Polymer Blends by DSC. Lecture at the Research Lab of the DuPont Co., Wilmington, DE, September 16.

Mesophases of Polymers. Invited Tutorial at the NATAS Meeting in Cincinnati, OH, September 22–24.

Thermal Analysis of PEEK. Contributed Paper at the NATAS Meeting in Cincinnati, OH, September 22–24.

A Personal Look at Macromolecular Science. Invited Presentations at the University of Tennessee, TN on September 25 and at Oak Ridge National Laboratories, Oak Ridge, TN on September 26. Theses were connected with extensive interviews and resulted in an offer of a position, as described on page 8-112.

[1986/87 Fourth Sabbatic, second in Germany. Organized with the help of Profs. Cantow (Univ. of Freiburg) and Pechhold (Univ. of Ulm), supported mainly by the Humboldt Prize (see page 8-111), including a follow-up visit in July/August 1988. The goal of the Sabbatic was to explore the various phases of matter as they represented themselves in form of mesophases and to work out a lecture series on Thermal Analysis, which gave the basis of a book in 1990 (Appendix A, #290). (Details in Chapter 8, pages 8-110–116, 8-121–122 and 8-124–129, Figures 100A–G and 102–108.)

Living in Schallstadt, near Freiburg, Im Zinken 2 bei Burggraf, followed by moving to Arnegg, near Ulm, Zeffler St. 11 bei Lusser, for the last 4 months. (Stay in both places with Heidel and Papa.)

1986, cont. Twenty lectures on Thermal Analysis. Lectures as a visiting professor at the University of Freiburg, Freiburg, Germany, October 14–December 16.

Der Starr-amorphe Zustand in Polymeren. Invited Lecture at the University of Mainz, Mainz, Germany, November 12.

Phasenumwandlungen in linearen Hochpolymeren. Invited Lecture at the University of Freiburg, Freiburg, Germany, November 25.

Thermoanalyse von linearen Hochpolymeren. Invited Lecture at the University of Basel, Basel Switzerland, December 17.

1987 *Return travel to the US to keep operations and lecturing commitments.*

Thermal Analysis of POM, PPO, and PPS. Lecture at the Research Laboratory of the DuPont Co. in Wilmington, DE, January 13.

Crystallization of Condis Materials. Lecture at the Research Laboratory of the Celanese Co. in Summit, NJ, January 14.

Crystallization of Linear Macromolecules. Teleconference of the Am. Chem. Soc., from home in Troy, NY, January 16. Travel back to Freiburg, January 30.

Analysis of Condis Crystals. Invited Lecture at the CRM, CNRS, Strasbourg, France, February 18.

Der starr-amorphe Zustand in semikristallinen Polymeren. Lecture at the BASF Research Laboratories, Ludwigshafen, Germany, February 25.

Kristallization von Polyäthylen und Paraffinen. Lecture at the Research Laboratory of Röhm, Darmstadt, Germany, February 26.

Der starr-amorphe Zustand in semikristallinen Polymeren. Lecture at the Makromolekular Kolloquium, Freiburg, Germany, March 12–14.

Fast, three-day turn-around trip to the APS Meeting in New York City

(A) The Rigid Amorphous State of Semicrystalline Macromolecules. (B) S. Z. D. Cheng and Computer Simulation of Motion on Crystal Surfaces and Molecular Nucleation of Macromolecules. (C) K. Loufakis and Heat Capacity of Liquid Linear Macromolecules. Three contributed lectures, In addition, the following five posters were presented: (D) D. Noid, Computer Simulation of 2-D Polymer Crystal Melting. (E) A. Xenopoulos, Thermal Properties of Polyamides. (F) M.-Y. Cao, Crystallization in Main-chain Mesogenic Polyesters. (G) G. A. Pfeffer, Static Simulation of Macromolecular Conformations on 2-D Surfaces. (H) H. S. Bu, The Tarasov Function in the Calculation of Heat Capacity. All given at the Am. Phys. Soc. Meeting in New York City, NY, March 16–19. (See page 8-119.)

(A) Die Thermoanalyse von PEEK. Contributed Paper, (B) Die Errechnung von Wärmekapazitäten fester Hochpolymerer aus Schwingungsspektren. Plenary Lectures, both at the Ulmer Kalorimetrietage, University of Ulm, Germany, March 23–24.

Wärmekapazitäten und Umwandlungen 1. Ordnung von Polymeren. Invited Lecture in the GEFTA, University of Tübingen, Germany, April 1–3.

1987, cont. Analysis of Condis Crystals. Invited Lecture at the 2nd Rolduc Meeting, Rolduc Abbey, The Netherlands, April 26–30.

Travel back to Troy to exchange winter to summer clothes and attend Brent's graduation in Syracuse,NY. (Travel with Heidel, see pages 8-82–83, 121.)

The Basis of Thermal Analysis. Lecture in a short course on Thermal Analysis at the Polytechnic Institute of New York, NY, May 12–13.

1987, cont. Thermoanalyse von Mesophasen. Invited Lecture at the Dechema Meeting in Frankfurt, Germany, May 14–15.

(A) Condis Crystals of Linear Macromolecules. (B) The Rigid Amorphous State of Linear Macromolecules. Two invited lectures at the Ciba/Geigy Research Labs in Fribourg, Switzerland, May 21–22.

Der Condis-Zustand in linearen Hochpolymeren. Invited Lecture at the University of Ulm, Ulm, Germany, May 25.

Der Condis-Zustand in kleinen Molekülen. Invited Lecture at the University of Ulm, Ulm, Germany, May 29.

Die Berechnung von Wärmekapazitäten von Hochpolymeren. Invited Lecture at the University of Ulm, Ulm, Germany, June 4.

Der starr-amorphe Zustand. Invited Lecture at the University of Ulm, June 19.

(A) Heat Capacity, Theory and Experiment. (B) Melting of Linear Macromolecules. (C) Mesophases of Linear Macromolecules. Invited lectures at the Thermische Analyse Werkgroep, Utrecht, The Netherlands, June 22.

Strukturen und Phasen in nieder- und hochmolekularen Molekülen. Invited Lecture at the University of Hamburg, Germany, June 23.

Condis State of Linear Macromolecules. Invited Lecture at the IUPAC Polymer Symposium, Merseburg, GDR, June 30–July 4 (see pages 8-124–128).

Der starr-amorphe Zustand von Hochpolymeren. Invited Lecture at the Technical University in Dresden, GDR, July 7.

Condis Mesophasen in Molekülen kleiner Masse. Invited Lecture at the Martin-Luther Universität Halle-Wittenberg, in Halle, GDR, July 9.

H. G. Wiedemann, Mesophase Transitions of Poly(diethyl siloxane). Contributed Lecture at the Int. Conf. on Liquid Crystals, Bordeaux, France, July 20–24.

Starr-amorphe Bereiche und Mesophasen in steifen und flexiblen Makromolekülen. Invited Lecture at Bayer, Leverkusen, Germany, August 3.

End of the Fourth Sabbatic.]

1987, cont. Condis Crystallinity in Polymers, especially PVDF. Invited Lecture at Pennwalt, King of Prussia, PA, August 25.

The Rigid Amorphous State in Textile Fibers. Invited Lecture at BASF-Enka, Enka, NC. September 11.

How to Grow Large Crystals of Linear Macromolecules. Invited lecture at the Akron Lecture Group, Akron, OH, October 7.

1988–2001 Knoxville, Tennessee

(See Chapter 9, UTK in Knoxville, TN and ORNL, 25 miles NW, see pages 9-4–5)

1988 200 Baltusrol Road, TN 37922-3707 (in 2005 the zip code changed to: **37934-3707**)
(See Chapter 8, Figure 109 and Chapter 9, Figure 1.)
[Professor and Distinguished Scientist at the University of Tennessee Knoxville (UTK), and at Oak and Ridge National Laboratory (ORNL).
(See Footnotes on pages 9-4 and 6); from January 1988, until retirement on June 1, 2001].

1988 Crystallization of Polyolefines. Invited Lecture at Milliken Chemicals, Spartanburg, NC, on February 17.

(A) Crystallization and Melting of Linear Macromolecules. (B) Glass Transition of Linear Macromolecules. Invited lectures at Asilomar Technical Conference on Polymer Thermal Characterization, Asilomar, Monterey, CA. March 3–8.

(A) S. Z. D. Cheng, The Principle of Molecular Segregation during Crystallization of PEO Fractions. (B) K. Loufakis, Conformational Disorder in Poly(vinylidene fluoride) as Studied by Thermal Analysis and on Molecular Mechanics Calculations of the Isolated Chain. (C) Conformational Motion and Disorder in Low and High Molecular Mass Crystals. (D) A. Xenopoulos, Conformational Disorder in Nylon 6,6. Four contributed lectures, and one poster: (E) H. S. Bu and S. Z. D. Cheng, Etching Methods to Study PEO Crystalline Morphology and Molecular Segregation, presented at the Am. Phys. Soc. Meeting in New Orleans, LA. March 20–24.

The Basis of Thermal Analysis. Lecture in a short course on Thermal Analysis at the Polytechnic Institute of New York, NY. May 9–11.

Trip to Italy, Germany, and Israel and spending the remaining month of the Humboldt stipend in Freiburg and Ulm
(With Heidel, for details of the trip see the listing on pages 9-20–22.)

The Rigid Amorphous State of Linear Macromolecules. Plenary Lecture at the First European Conference on Advanced Topics in Polymer Science. Polymer Crystals. Gargnano, Italy. June 19–24.

Die Probleme der Kristallisation von Polymeren, diskutiert am Beispiel des Polyäthylenoxyds. Colloquium at the University of Freiburg, Freiburg, Germany. July 12.

*S. Z. D. Cheng, Kinetic Study of Mesophase Transitions. Poster, presented at the third Gordon Research Conference on Liquid Crystalline Polymers, New London, NH. July 10–15.

Beispiele von starr–amorphen Polymeren. Invited Lecture at the University of Freiburg, Freiburg, Germany. July 15.

Die Thermoanalyse von Polydiethylsiloxan. Seminar at the University of Ulm, Ulm, Germany. July 26.

Beispiele von starr-amorphen Polymeren. Invited Lecture at the Research Laboratory Farbwerke Höchst, Frankfurt-Höchst, Germany. August 2.

Die Probleme der Kristallisation von Polymeren, diskutiert am Beispiel des Polyäthylenoxyds. Seminar at the Research Laboratories of the BASF in Ludwigshafen, Germany. August 4.

Thermal Analysis of Conformational Disorder in Small and Large Molecules. Invited Lecture at the Max Planck Institut in Stuttgart, Germany. August 5.

The Detection of Conformational Disorder by Thermal Analysis. Plenary Lecture at the 9th International Congress on Thermal Analysis in Jerusalem, Israel. August 21–25.

S. Z. D. Cheng, Thermal Analysis of Thermoplastic Polymers. Contributed Lecture at the 9th International Congress on Thermal Analysis, Jerusalem, Israel. August 21–25.

The Advanced THermal Analysis System. Plenary Lecture at the Penn State Symposium on Polymer Characterization, Penn State University, State College, PA. October 16–19.

How to Fit Large Molecules and Mesophases into the Scheme of General Chemistry. (A) Invited seminar at the Department of Chemistry of the University of Toledo, Toledo, OH. October 26 and (B) the Department of Chemistry and Chemical Engineering of Northern Michigan Institute of Technology, Houghton, MI. October 27.

Thermal Analysis and Molecular Mechanics Calculation for Condis Crystals with Main- and Side-chain Conformational Disorder. Contributed lecture at the Annual Materials Research Society Meeting in Boston, MA. November 27–December 2

Second Travel to Italy (Accompanied by Heidel.)

1988, cont. The Rigid Amorphous State in Semicrystalline Macromolecules. Invited Seminar at the Department of Industrial Chemistry of the University of Genoa, Italy. December 9.

The Detection of Conformational Disorder by Thermal Analysis. Plenary Lecture at the Xth Convegno Nazionale Assoc. Ital. di Calorimetria ed Analysi Termica (AICAT) in Pisa, Italy. December 11–14.

1989 Conformational Disorder in Small and Large Molecules. Invited Lecture at the Department of Polymer Science of the University of Akron, Akron, OH. January 5.

Crystallinity of Macromolecules. Invited Lecture at the Firestone Research Center in Akron, OH. January 6.

Thermal Analysis of Linear Macromolecules. Invited Lecture at the Akron Polymer Lecture Group. Akron, OH. January 6.

Consulting visit in Darmstadt, Germany

Diskussion und Beratung über Zusatzmittel für die Beeinflussung der Morphologie von Paraffinkristallen. Lecture at the Zentrallabor der Chemischen Werke Röhm, Darmstadt, Germany. March 7.

1989, cont. Makromolekulare Kondiskristalle. Plenary Lecture at the Makromolekularen Kolloquium an der Universität Freiburg, Germany. March 9–11.

(A) Main-chain and Side-chain Conformational Disorder. (B) M. Varma-Nair, The New ATHAS Laboratory. Two contributed lectures and (C) M. Yasuniva, High Pressure Crystallization of Polyethylene. (D) A. Xenopoulos and K. Roles, Heat Capacities of Polypeptides and Proteins. (E) B. G. Sumpter and D. W. Noid, Molecular Dynamics Simulation of the Melting Transition of Polyethylene. (F) Y. Yin, Single Run Heat Capacity Measurement. Four posters at the Am. Phys. Soc. Meeting in St. Louis, MO. March 19–24.

The Basis of Thermal Analysis. Feature lecture in a course on Thermal Analysis at the Polytechnic Institute of New York, NY. May 8–10.

*B. G. Sumpter and D. W. Noid, Computer Simulations in Polymers: Conformational Disorder, Spectra, Heat Capacities, Laser Interactions, Chemical Reactions, and Melting Transition. Seminar at the Departmento de Quimica Fisica, Facultad de Clencias Quimicas, Universidad Complutense de Madrid, Spain. May 19.

Conformational Disorder and Motion in Small and Large Molecules. Invited lecture at the Research Center of Tennessee Eastman, Kingsport, TN. May 22.

*B. G. Sumpter and D. W., Noid, Computer Simulations of Polymer Dynamics. Invited lecture at the IX International Conference on Computers in Chemical Research and Education. Riva Del Garda, Italy. May 28–June 2.

*B. G. Sumpter, D. W. Noid, Molecular Dynamics Studies of the Degradation of Polymer Surfaces: Laser Ablation and Collisional Energy Transfer. Poster at the Gordon Conference on Molecular Energy Transfer, Wolfeboro, NH. July 2–7.

Visit to Germany (Travel with Heidel, including a week's vacation in Kössen.)

1989, cont. Simulation von Polymerkristallen zur Ermittlung der Konformations-unordnung, Anharmonizität, und Wärmekapazität. Five invited lectures at (A) the University of Hamburg, Germany. July 4; (B) the University of Ulm, Germany. July 7; (C) the Max-Planck-Institut für Festkörperforschung in Stuttgart, Germany. July 17; (D) the Max-Planck-Institut für Polymer-forschung in Mainz. Germany. July 18; and (E) the University of Freiburg, Germany. July 26.

Determination of Molecular Disorder and Motion by Thermal Analysis. Invited Lecture at the Gordon Conference on Analytical Chemistry, New Hampton, NH. August 6–11.

*B. G. Sumpter, D. W. Noid, Computer Simulation of Polymer Dynamics in the Solid Phase. Invited lecture at the ACS National Meeting, Symposium on Computer Simulation of Polymer Dynamics, Miami, FL. September 10–15.

Conformational Disorder and Motion in Small and Large Molecules. Invited lecture at the Research Center of Proctor and Gamble, Miami Valley, Cincinnati,

OH. September 25 and the Research Center of the Shell Development Co., Analytical Division, Houston, TX. October 2.

1989 cont. B. G. Sumpter, Theoretical Studies of the Dynamics of Polymers in the Solid State. Invited Seminar at the Materials Science Department of the University of Tennessee in Knoxville, TN. October 5.

Physical Chemistry of Linear Macromolecules. Two invited lectures at (A) the Bob Johnes University, Greenville, SC. October 10 and (B) the Wofford College, Spartanburg, NC. October 30.

1990 Conformational Disorder in Nylons. Contributed lecture and (B) B. G. Sumpter, D. W. Noid, S. Z. D. Cheng, Computer Simulations of Polymer Phase Transitions: Conformational Disorder. (C) D. W. Noid, B. G. Sumpter, Molecular Dynamics Calculation of the Density of States for Polyethylene: Collective vs. Local Modes. (D) G. A. Voth, B. G. Sumpter, D. W. Noid, Infrared Laser Induced Phase Transitions and Ablations in Polymer Crystals. Three posters at the APS Meeting in Anaheim, CA. March 11–16.

Molecular Dynamics Simulation of Macromolecular Crystals. Invited Lecture at the Dept. of Chemistry, Rensselaer Polytechnic Institute, Troy, NY. March 24.

Molecular Motion in Polymers Studied by Supercomputers and Calorimetry. Invited lecture at the University of Massachusetts, Amherst, MA. April 6.

The Heat Capacity of Rigid and Amorphous Phase Macromolecules. Invited tutorial at the Am. Chem. Soc. Meeting, Boston, MA. April 23–27.

Travel to the Netherlands (Together with Heidel.)

Molecular Dynamics Simulation and Thermal Analysis of Polymer Crystals. Invited review lecture at 5th Fifth Rolduc Meeting on Integration of Fundamental Science and Technology. Rolduc, Kerkrade, Netherlands. April 29–May 3.

The Heat Capacity of Rigid and Amorphous Phase Macromolecules. Invited lecture at the Research Center of DSM at Geleen, The Netherlands, on May 4.

(A) *D. W. Noid, B. G. Sumpter, Molecular Dynamics Computer Simulations of Spectra and Structure of Polymers. (B) *B. G. Sumpter, D. W. Noid, Computer Experiments on the Internal Dynamics of Crystalline Polyethylene: Mechanistic Details of Conformational Disorder. Two invited lectures at the Akron Polymer Conference, Akron, OH. May 14–15.

(A) *A. Xenopoulos, On the Brill Transition of Nylon 6.6. Contributed lecture at the Int. Disc. Meeting on Relaxation in Complex Systems. Heraklion, Crete, Greece. June 18–29. (B)*A. Xenopoulos, J. Cheng, M. Yasuniva, Solid State Transitions of Ammonium Salts. (C) *A. Xenopoulos, A. H. Narten, X-ray and Neutron Scattering Studies of Semicrystalline Nylons. (D) *A. Xenopoulos, D. W. Noid, B. G. Sumpter, Generation and Correlation of Rotational Isomers in Polyethylene-like Crystals. Four contributed lectures at the Int. Disc. Meeting on Relaxation in Complex Systems. Heraklion, Crete, Greece. June 18–29.

1990 cont. Mesophase Crystals (Structure, Texture, Motion and Order in Liquid Crystals and Condis Crystals). Invited Tutorial at the Shell Development Co. Westhollow Research Center, Houston, TX. June 7.

The Condis Phase, A Mesophase for Macromolecules. Poster at the Gordon Conference on Liquid Crystals, New London, NH. July 2–6.

M. Varma-Nair, Data Bank and Computation of C_p, H, S, and G. Contributed lecture and at the 33rd IUPAC Macromolecular Symposium in Montreal, Canada. July 8–13.

Travel to Lake Como, Italy (With Heidel.)

Gradual Transitions to Conformational Disorder in Molecular Crystals. Invited lecture at the 11th IUPAC Conference of Chemical Thermodynamics, Como, Italy. August 26–31.

The Advanced THermal Analysis System (ATHAS) for Polymers. Plenary lecture at the Union Carbide Analytical and Physical Measurements Symposium. Parma Technical Center, Parma OH. September 19.

(A) Thermal Analysis and Simulation by Supercomputer of the Crystal-to-Condis-Crystal Transitions in Polyethylene. (B) J. Grebowicz, Thermal Properties of Drawn Polytetrafluoroethylene. Contributed lectures to the 19th NATAS Conference, Cambridge, MA. September 23–26.

The Heat Capacity of Rigid Crystalline and Amorphous Macromolecules. Invited lecture at the University of Southern Mississippi Polymer Symposium Series. Hattiesburg, MS. October 3.

Third travel to Japan (See also page 9-55 and Figure 55 in Chapter 9.)

Analysis and Prediction of Thermal Properties of Mesophases and Crystals by Calorimetry and Supercomputers. Plenary lecture at the 11th Conference of The Association for the Progress of New Chemistry (of Japan) at Shuzenji, Japan. November 6–9.

(A) D. W. Noid and B. G. Sumpter, Molecular Dynamics Simulation of Polymer Crystals. Poster, and (B) Defect Generation and Motion in Polyethylene-like Crystals, Analyzed by Simulation with Supercomputers. Materials Research Society, Contributed Paper, Boston, MA. November 26–December 1.

1991 (A) Defects in Polyethylene; (B) D. W. Noid, B. G. Sumpter, J. A. Darsey, Molecular Dynamics Simulation of Crystalline Polymers; (C) K. A. Roles, Heat Capacities of Solid Poly(amino Acid)s; (D) M. Varma-Nair, High Temperature Transitions in Poly(oxy-1,4-phenylenecarbonyl-*co*-oxy-2,6-naphthaloyl); (E) A. Xenopoulos, A. H. Narten, Proton Motion in Semi-crystalline Nylons from Neutron Scattering; a record in numbers of presented lectures at an APS Meeting, supported by five posters: (F) G. L. Liang, D. W. Noid, B. G. Sumpter, Molecular Dynamics Simulation of Electric Field Induced Defects in Polyethylene; (G) Y. Jin, Heat Capacity of *n*-Paraffins

and Polyethylene; (H) J. Cheng, Study of Molecular Motion in Tetra-*n*-alkyl Ammonium Halides by NMR; (I) B. Annis, D. W. Noid, B. G. Sumpter, J. Reffner, Applications of Atomic Force Microscopy to Polymer Samples; (J) A. Habenschuss, A. Xenopoulos, X-ray Diffraction Studies of Aliphatic Nylons; (K) G. Pfeffer, B. G. Sumpter, D. W. Noid, Infrared Laser Induced Chaos and Conformational Disorder in Polymer Crystals; all lectures were presented at the American Physical Society Meeting in Cincinnati, OH, on March 18–21. The different first authors indicate that 10 members of the ATHAS/ORNL group attended the meeting (see Chapter 9, Figure 40).

1991 cont. (A) *D. W. Noid, b. G. Sumpter, J. A. Darsey, Molecular Dynamics Simulation of Crystalline Polymers. (B) *C. Getino, B. G. Sumpter, D. W. Noid, Internal Energy Migration in Polymer Crystals; (C) *B. G. Sumpter, C. Getino, D. W. Noid, A. Xenopoulos, Computational Studies of Submicron Probing of Polymer Surfaces. Three papers at the 201st National ACS Meeting, Atlanta GA, April 15–19.

Molecular Dynamics Simulation and Thermal Analysis of Macromolecular Crystals. Invited lecture at the Meeting of the Midwest Thermal Analysis Forum, Minneapolis, MN, April 17.

*A. Xenopoulos, Thermal Analysis of Aliphatic Polyamides. Seminar, given at the Polytechnic University, Barcelona, Spain, April 26.

The Basis of Thermal Analysis. Feature lecture in a short course on Thermal Analysis by the Polytechnic University of New York, held in Park Ridge, NJ. April 29–May 1.

*B. G. Sumpter, D. W. Noid, Nonlinear Resonances and Chaos in Polyethylene. Lecture at the ACS Joint Central-Great Lakes Regional Meeting, Indianapolis, IN, held in May.

Traveling to Stockholm, Sweden, followed by the first trip to a unified Germany. (With Heidel, see pages 9–30–33 and Figures 22–27 of Chapter 9.)

A Review of Phase Transitions involving Mesophases. Plenary lecture at the 23rd Europhysics Conference on Macromolecular Physics in Stockholm, Sweden, May 26–31.

*A. Xenopoulos, Simulation of the Dynamics of Crystals of Polyethylene. Seminar at the Department of Chemical Engineering, Polytechnic University of Catalonia, Barcelona, Spain, May 30.

Simulation der Molekulardynamic und der thermischen Analyse bei Polymerkristallen. Seminar at the Technical University of Berlin (Berliner Polymeren Colloquium), Germany, June 4.

Molecular Dynamics Simulation and Thermal Analysis of Macromolecular Crystals. Invited lectures at (A) the Bundesanstalt für Materialprüfung, Berlin, Germany, June 5 and (B) the Institutscolloquium at the Physikalisch Chemische Institut, Humboldt University, Berlin, Germany, June 6.

1991 cont. *A. Xenopoulos, X-ray and Neutron Scattering of Polyamides. Seminar at the Laboratory of Solid State Physiscs, University Paul Sabatier, Toulouse, France, June 7.

News from ATHAS (Atomic Force Microscopy, Solid State NMR, and Calorimetry in the Study of Macromolecular Crystals). Invited Colloquium at the Institut für Makromolekulare Chemie, University of Freiburg, Germany, June 12.

Molecular Dynamics Simulation and Thermal Analysis of Macromolecular Crystals. Lecture at the Physical and Analytical Division of Tennessee Eastman, Kingsport, TN, June 20.

*A. Xenopoulos, Thermal Analysis and Neutron Scattering of Nylon 6 and Nylon 6,6. Seminar at the Institut für Makromolekulare Chemie, University of Freiburg, Freiburg, Germany, July 2.

A. Xenopoulos, Defects in Aliphatic Polyamides. Seminar at the Department of Materials Science and Engineering at the University of Tennessee, Knoxville, TN, September 5.

New Directions in Thermal Analysis. Plenary lecture at the North American Thermal Analysis Soc. Meeting in Minneapolis, MN, September 23–26

Travel to Wageningen in The Netherlands

(A) New Directions in Thermal Analysis, and (B) The Athas System at the University of Tennessee. Invited lecture at the 25th Annual Meeting of the Thermal Analysis Workgroup of the Netherlands, Wageningen, The Netherlands, October 1–2.

Detection of Disorder by Thermal Analysis. Seminar at the Department of Materials Science and Engineering at the University of Tennessee, Knoxville, TN, October 31.

Differential Thermal Analysis: Instrumentation and Interpretation. Eastern Analytical Symposium. Featured Lecture, Somerset, NJ. November 11–15.

1992 Characterization of the Glass Transition by Thermal Analysis. Invited lecture, Fifth Analytical Symposium of the Hercules Co. Wilmington, DE., January 22–23.

Thermodynamics of Fullerene. Seminar at the Chemistry Division of ORNL, Oak Ridge, TN, January 29.

Thermodynamics of Macromolecular Crystals. Invited lecture, Dept. of Chemistry, West Kentucky University, Bowling Green, KY, February 7.

(A) Unfreezing of Large-amplitude Motion in Polymers; (B) Distinction between Liquid Crystals, Plastic Crystals, and Condis Crystals. Two invited lectures at the Research Laboratory of the Shell Development Co. in Westhollow, TX., February 18.

(A) Defects in Polyethylene; (B) D. W. Noid, B. G. Sumpter, M. Varma-Nair and J. Darsey, Neural Network Simulations of Chemical Systems; (C) A. Xenopoulos, J. Cheng, A. Habenschuss, Distinction between Plastic and Condis Crystals of Tetra-*n*-alkylammonium Salts; three contributed lectures,

and: (D) J. Cheng, Y. Jin, Solid State C-13 NMR Studies of Molecular Motion in MBPE-9 and MBPE-5; (E) G. L. Liang, D. W. Noid, and B. G. Sumpter, Molecular Dynamics Simulation of Phase Transitions in Polyethylene; (F) Y. Jin, J. Cheng, Thermodynamic Properties and Motion in MBPE; (G) Y. Fu, Y. Jin, W. Busing, Full-pattern X-ray Diffraction and Thermal Analysis Study of Poly(ethylene terephthalate) Fibers; (H) A. Habenschuss, A. Xenopoulos, Structural Changes in Mesophase Transitions of Tetra-*n*-alkylammonium Halides; (I) J. Cheng, A. Xenopoulos, Solid State NMR Study of Orientational and Conformational Motion and Disorder in Tetra-*n*-alkylammonium Halides; (J) A. Habenschuss, M. Varma-Nair, X-ray Diffraction Study of Poly(oxybenzoic acid), POB, Poly(oxynaphthoic acid), PON, and their Copolymers; (K) M. Varma-Nair, D. W. Noid, Neural Network Prediction of Heat Capacities of Macromolecules. (L) G. A. Pfeffer, B. G. Sumpter, G. L. Liang, Chaotic Dynamics and Conformational Change in Ultraoriented Polyethylene; eight posters at the Am. Phys. Soc. Meeting in Indianapolis, IN, March 15–20. Again, at this meeting 10 members of ATAHAS/ORNL were attending, as in 1991 (see Chapter 9, Figure 40).

1992 cont. The Basis of Thermal Analysis. Invited Lecture, Thermal Analysis Short Course of the Polytech. Univ. of New York in Park Ridge, NJ, April 27–29.

Travel to Sweden for a lecture series at the Kgl. Technical University (With Heidel.)
A course of seven 90 min lectures on the "The Condensed State of Linear Macromolecules." (Crystal Structure I; II; Crystal Morphology; Defects in Polymers; Transitions; Mesophases; and Melts and Glasses). Kgl. Technical University, Stockholm, Sweden, June 1–5. (See page 9-39.)

Molecular Dynamics Simulation and Thermal Analysis of Macromolecular Crystals. Plenary Lecture at the 13th Nordic Symposium on Thermal Analysis and Calorimetry. Stockholm, Sweden, June 9–11.

Defects in Polyethylene. Invited Lecture at the Research Laboratorium of the BASF in Ludwigshafen, Germany, June 16.

Computer Simulation of Polymer Crystals. Invited Lecture, Gordon Conference on Polymers, Brewster Academy Wolfeboro, NH, June 28 July 3, 1992.

Thermotropic Polymer Mesophases with Missing Entropies of Transition. Invited Lecture at the Gordon Conference on Liquid Crystals of Polymers, Colby Sawyer College, New London, NH, July 5–10.

*Y. Fu, Y. Jin, K. Affholter, W. Busing, Full-pattern (2-D Rietveld) X-ray Diffraction Studies of Poly(ethylene terephthalate) Fibers. Lecture at the 41st Annual Denver X-ray Conference, Colorado Springs, CO, August 3–7.

(A) The Thermodynamic Functions of Poly(amino acid)s and Proteins. (B) Measurement of Changing Conformational Disorder in Solids Outside the Transition Region by Calorimetry. Contributed lectures, 12th IUPAC Conference on Chemical Thermodynamics in Snowbird, UT, August 16–21.

Travel to the 2nd International Meeting on Polymer Crystallization (With Heidel.)

1992 cont. Unsolved Problems of Crystallization of Flexible Macromolecules. Attempts at the Understanding of the Molecular Process by Experiments and Computer Simulation. Invited Lecture at the NATO Workshop on Polymer Crystallization in Mons, Belgium, September 6–12. (See page 8-63)

(A) A. Xenopoulos, Thermal Analysis of Alkylammonium Salts; (B) Y. Jin, Single Run Heat Capacity Measurement by DSC: Principle, Experimental Detail and Data Analysis. Two contributed lectures and (C) Y. Jin, Y. Fu, M. Mucha, Thermal Characterization of Poly(ethylene terephthalate); three posters and: (D) M. Varma-Nair, A. Habenschuss, Phase Transitions in Poly(4-hydroxybenzoic acid), Poly(2,6-hydroxynaphthoic acid) and their Copolymers. (E) M. Varma-Nair, Thermal Analysis of Epoxy Resins. (F) Thermal Properties of the Three Allotropes of Carbon; three contributed lectures at the North American Thermal Analysis Society Conference (NATAS) in Atlanta, GA, September 13–16.

Travel to South Africa to Lecture at the SATAS Meeting (Accompanied by Heidel, see pages 9-57–59 and Figures 60 and 61 in Chapter 9.)

The Presence and Future of Chemical Industry. Discussion at the Plastic Federation of South Africa, Johannesburg, SAR, October 26.

Determination of Molecular Mass and Crystallinity of Polytetrafluoroethylene. Invited lecture, Atomic Energy Corp. of SA, Pretoria, SAR, October 30.

New Directions in Thermal Analysis. Plenary lecture at the South African Thermal Analysis Society Meeting, SATAS, in Pretoria, SAR, November 2–3.

(A) The Theory and Practice of Measurement of Heat Capacity; (B) The Microscopic Link Between Thermal Properties and Molecular Structure; (C) The Link Between Thermal Properties and Molecular Structure; (D) The Measurement, Classification, Interpretation, and Prediction of Phase Transitions. Four invited Lectures at the SATAS Meeting in Pretoria, SAR, Werkswinkel oor warmtekapasiteitsbepalings en die termodinamiese belangrikheid daarvan, November 2–3.

The Basis of Thermal Analysis and the Advanced Thermal Analysis System. Invited Lecture at the SASOL Research Facility, Sasol, SAR, November 4.

The Industrial Handling of Nylons. Discussion at the SA Nylon Spinners, Capetown, SAR, November 6.

Fourth Travel to Japan (Accompanied by Heidel, see page 9-55.)

The Defect State of Macromolecules in Crystals and Mesophases as Analyzed by Calorimetry, Supercomputer Molecular Dynamics Simulation, and Solid State NMR. Invited Lecture, 4th International Meeting of the Society of Polymer Science of Japan in Yokohama, Japan, November 29–December 3.

Defects in Polyethylene. Invited Seminar at Gunma University in Kiryu City, Japan, December 4.

1993 Polymer Films and their Analysis. Invited Lecture at the research facility of Medtronics Co. in San Diego, CA, January 29.

The Nature of the Glass Transition and its Determination by Thermal Analysis. Opening Lecture at the ASTM Meeting on The Assignment of the Glass Transition in Atlanta, GA, March 3–5.

*Y. Jin, A. Boller, Heat Capacities and Transitions in Perfluorinated Paraffins and Poly(tetrafluoethylene). Contributed Lecture to Pitcon'93, Atlanta, GA, March 8–11.

(A) Analysis of the Hexagonal Phases of Polymers and Oligomers; (B) C. E. Wozny, B. G. Sumpter, D. W. Noid, Vibrational Analysis of Random Coil Polyethylene; (C) A. Xenopoulos, Y. Jin, M. Diak, G. Guichon, R. N. Compton, Thermodynamic Properties of C70; (D) A. Xenopoulos, K. Roles. A Possible Glass Transition for Poly(L-methionine) and Poly(L-serine); Four contributed lectures, and (E) A. Xenopoulos, T. Habenschuss, A. H. Narten, X-ray Studies of Symmetric Tetra-*n*-alkylammonium Halides; a poster at the American Physical Society Meeting in Seattle, WA, March 22–26.

The Basis of Thermal Analysis, Invited lecture at the 17th Symposium on Thermal Analysis of New York Polytechnic University, held at Park Ridge, NJ, April 19–21.

Production of Single-molecule Phases in Microgravity. Invited lecture at the Workshop on Organic and Polymeric Materials, NASA, Huntsville AL, April 27–28.

Solid State Physics of Polymers. Seminar at Rennsselaer Polytechnic Institute, Troy, NY, May 10.

*(A) Y. Fu, W. R. Busing, and K. A. Affholter, Full-pattern Refinement of Poly(ethylene terephthalate) fibers; poster and *(B) A. Xenopuoulos, A. Habenschuss, X-ray Diffraction Studies of Mesophase Transitions in Homologous Series of Symmetric Tetra-*n*-alkylammonium Halides; lecture contributed to the Am. Cryst. Assoc.'93 in Albuquerque, NM, May 23–27.

Fifth trip to Japan (Accompanied by Heidel, see page 9-56 and Figures 56–57.)

Computer Simulation of Macromolecular Crystals and their Defects. Invited lecture at the Osaka University International Macromolecular Symposium (to recognize the 30 Year Anniversary of the Department of Macromolecular Science of the University of Osaka) on "Ordering in Macromolecular Systems," Osaka, Japan, June 3–6.

The Rigid Amorphous Fraction of Crystalline Polymers. A two-lecture series and discussion at the research laboratory of the Toray Research Center in Otsu, Japan, June 7.

Thermal Analysis of Mesophases. Seminar at the University of Osaka, Osaka, Japan, June 10.

1993 cont. The Three Phases in PET Fibers, Analyzed by Thermal Analysis and X-ray Diffraction, invited lecture, and Y. Fu, A. Boller, and Y. Jin, X-ray Diffraction of Super-drawn Polyethylene Fibers, poster. Both presented at the Fibers Gordon Conference in New London, NH, July 11–16.

Heat Capacities of C_{60}, C_{70}, and C_{70} $C_6H_5CH_3$ and their Transitions. Contributed lecture to the Calorimetry Conference, Durham, NC, July 19–22.

Travel to receive the Swiss Prize for Applied Chemical Thermodynamics
(Thereafter joined by Heidel and Caryn for a vacation in Kössen.)

Thermodynamische Charakterisierung von Mesophasen. Awards Lecture at the joint German Society for Thermal Analysis (GEFTA) and the Swiss Society for Thermoanalytic and Calorimetry (STK), Munich, Germany, September 13–15. (See pages 9-18 and 19)

*Y. Jin and A. Boller, Heat Capacity Measurement by Modulated DSC. Contributed Lecture at the 22nd Annual North American Thermal Analysis Society Meeting, NATAS, in Denver, CO, September 19–24.

Glass Transitions of Partially Ordered Macromolecules. Invited Lecture at the 28th Europhysics Conference on Macromolecular Physics, Ulm, Germany, September 27–October 1.

The Three Phases in PET Fibers, Analyzed by Thermal Analysis and X-ray Diffraction. Seminar at the Materials Engineering Dept., University of Tennessee, Knoxville, October 14.

Defects in Polyethylene. Invited Lecture at the EXXON Research Company in Linden, NJ, November 19.

(A) Thermal Properties of Fullerenes; invited lecture and (B) Atomistic Details of the Disordering Process in Superheated Polymethylene Crystals. (C) A. Xenopoulos, M. Mucha, Nonequilibrium States of Symmetric Tetraalkylammonium Halides; Three contributed lectures, and (D) A. Xenopoulos, J. D. Londono, and G. D. Wignall, Phase Separation in Polystyrene-Poly(*p*-methylstyrene) Blends Using Thermal Analysis and Small Angle Neutron Scattering; (E) Thermal Properties and Motion in C_{60}, C_{70}, and the $C_{70}{\cdot}C_6H_5CH_3$-Complex as Analyzed by DSC and NMR; two posters at the Material Research Society, Fall Meeting in Boston, MA, November 28–December 3.

1994 (A) J. Cheng, M. Fone, Solid State 13C NMR Study on the Intermediate Phase and Domain Sizes of Polyethylene; (B) Remarks on Gradual Change of Conformational Disorder; Two lectures and (C) J. Cheng, Y. Jin, W. Chen, The Chain Conformation of a Polyester Based on Bis(4-hydroxyphenoxy)-*p*-xylylene and 1,11-Dibromoundecane (HPX-C11) and its Mesophase States; (D) A. Habenschuss, M. Varma-Nair, The Phase Diagram of Copolymers of 4-Hydroxybenzoic Acid and 2,6-Hydroxynaphthoic Acid from X-ray Diffraction and Thermal Analysis; (E) Q. Wang, B. Annis, A. Habenschuss, Investigation of the Surface Structure in Tetraalkyl Ammonium Halides by

Atomic Force Microscopy; (F) G. Liang, D. Noid, B. Sumpter, Molecular Dynamics: Effects of Surface-constraints on the Crystal Structure, Phase Transition, Defect Distribution, Mass Transport, and Surface Melting in Polymethylene; (G) A. Boller, B. Annis, Three-phase Structure-Property Analysis of PET Fibers. (H) Y. Fu, B. Annis, A. Boller, Structure Analysis of High-modulus Polyethylene Fibers Using a Three-phase Model; (I) W. Chen, Investigation of Polyethylene Fibers by Solid State NMR; seven posters at the American Physical Society Meeting in Pittsburgh, PA, March 21–24. After a smaller showing at the 1993 APS Meeting in Seattle (due to the long distance to travel), again, a delegation of eight members of the ATHAS/ORNL Polymer Group could present their work in Pittsburgh.

1994 cont. The Basis of Thermal Analysis. Invited lectures, 18th Thermal Analysis Symposium, at the Polytechnic University of New York, at Park Ridge, NJ, April 18–20.

The Crystal Morphology, Macroconformations and Defects of Polyethylene. Tutorial at the RayChem Research Laboratory, Menlo Park, CA, April 29.

The Defect State of Polymers Analyzed by Calorimetry, Solid State NMR and Molecular Dynamics Simulation. Seminar at the RayChem Research Laboratory, Menlo Park, CA, April 29.

Travel to England and Germany, 3rd Lähnwitz Seminar (With Heidel, see page 9-34.)

Molecular Motion in Polymers Simulated by Supercomputer and Measured by Calorimetry. Invited lecture, and Modulated Differential Scanning Calorimetry, a seminar at the ICI Paints Research Laboratory, Slough, Berkshire, England, May 23.

The Defect State of Polymers, Analyzed by Calorimetry, Solid State NMR, and Molecular Dynamics Simulation. Lecture at the ICI Research Laboratory in Wilton, England, May 24.

The Advanced Thermal Analysis System (ATHAS). Keynote Lecture at the meeting on 'The Application of Differential Scanning Calorimetry to Physical Characterization of Polymers' of the Royal Society of Chemistry, Society of Chemistry Industry and Analytical Division (Thermal Methods Group). London, England, May 26.

Crystallization During Polymerization. Lecture at the Shell Development Laboratories in Amsterdam, The Netherlands, May 31.

(A) Modulated DSC—Capabilities and Limits. Invited Lecture at the 3rd Lähnwitz Seminar about "Bestimmung von Umwandlungsenthalpien" and (B) A. Boller, "Bestimmung von Umwandlungsenthalpien außerhalb des Umwandlungsbereiches," poster. Serrahn, Germany, June 2–4. (Material for both contributions is given in publications 378 and 385 of Appendix A).

*A. Boller, Temperature-modulated DSC. Seminar at the Department of Physics, University of Rostock, Rostock, Germany, June 10.

1994 cont. *A. Boller, Temperature-modulated DSC. Colloquium at the Sektion für Kalorimetrie, Dept. of Physics, University of Ulm, Ulm, Germany, June 20.

(A) Large-amplitude Motion in Polymer Crystals and Mesophases. (B) Single-chain Single-crystals, invited lectures at the 35th IUPAC International Symposium on Macromolecules, MacroAkron '94, Akron, OH, July 11–15.

IUPAC International Symposium on Thermochemistry in France (With Heidel.)

The ATHAS Data Bank of Heat Capacities of Linear Macromolecules. Plenary Lecture at the IUPAC International Symposium on Thermochemistry, Clermont-Ferrand, France, July 17–22.

*Y. Fu, and B. Annis, Two-dimensional Rietveld Refinement Studies of Fibers. Lecture at the 43rd Annual Denver Conference on Applications of X-ray Analysis. Steamboat Springs, CO, August 1–5.

(A) Thermal Analysis Instrumentation for the Measurement of Transitions in Polymers. (B) The Glass Transitions and Disordering Transitions in Polymers. Two Tutorials in connection with the 23rd NATAS Conference in Toronto, Canada, September 24–28.

The Measurement of the Glass Transition with Modulated DSC and its Relation to Dynamic Mechanical and Electrical Analyses. Contributed lecture at the 23rd NATAS Conference in Toronto, Canada, September 24–28.

Sixth Trip to Japan (Accompanied by Heidel, see page 9-56.)

Gradual Change of Conformational Disorder. Invited Lecture at the International Polymer Physics Symposium Honoring Professor Torhu Kawai's 70th Birthday, Tokyo, Japan, October 25–25.

Large-amplitude Motion in Polymer Crystals and Mesophases. Seminar at the University of Hiroshima, Higashi-Hiroshima, Japan, October 26.

Large-amplitude Motion in Polymer Crystals and Mesophases. Invited Lecture at the International Symposium on Polymer Crystallization, in Gakunan, Okayama, Japan, October 28–29.

New observations about Phase Transitions. Seminar at the Department of Chemistry, University of Tennessee, Knoxville, TN, December 8.

1995 The Energetics and Defects of Paraffins. Discussion at the Exxon Research Laboratory, Linden, NJ, January 23.

Defects in Polymer Crystals. Seminar at the Department of Materials Science, University of Illinois, Urbana, IL, January 30.

(A) A. Boller, Glass Transition Determination by Modulated DSC; (B) Multiphase Structures in Fibers; (C) G. Zhang, Heat Capacities of Polymers; Three lectures and (D) M.Pyda, W. Chen, Study of the Mesophase of PEIM-12 by Thermal Analysis; (E) W. Chen, M. Pyda, Study of the Mesophase of PEIM-12 by Solid State 13C NMR; (F) Y. Fu, Structure Analysis of Poly(*p*-phenylene terephthalamide) Fibers with Full-pattern X-ray Diffraction

Method; three posters at the Am. Phys. Soc. Meeting, San José, CA, March 20–24. As usual, the West Coast Meetings saw a smaller attendance from us.

1995 cont. Nonequilibrium of Crystallization, Annealing, and Melting. Lecture at the Cygnus Research Laboratory, Redwood City, CA, March 24.

Defects in Polymer Crystals, invited lecture in the PMSE Symposium, and The Difference between Liquid Crystals and Conformationally Disordered Crystals, invited lecture in the Polymer Div. Symposium on "Processing-Structure-Property Relationships in LCP," both at the Am. Chem. Soc. Spring Meeting in Anaheim, CA, April 2–7.

Modulated DSC, Featured Lecture at the Golden Gate Polymer Forum in San José, CA, April 10.

Beginning to Understand the Strongest Materials (Polymer Fibers). Lecture at the MRS Seminar at the University of Tennessee, April 12.

Defects in Polymer Fibers. Seminar at the Höchst-Celanese Research Lab in Summit, NJ, April 24.

(A) Thermodynamic Functions and Modulated Calorimetry; (B) Phase Transitions; two lectures at the 19th Annual Short Course on Thermal Analysis in Polymer Research and Production, Polytechnic Polymer Research Institute, given at Park Ridge, NJ, April 24–26.

Modulated DSC of Polymers, and Phase Structure and Transitions of Semicrystalline Polymers. Two lectures at the Shell Development Co. Westhollow Research Center, Houston, TX, May, 15.

Travel to Regensburg Germany (Together with Heidel.)

Der Defektzustand in Polymerkristallen. Colloquium at the Physics Department of the University of Regensburg, Germany, June 19.

*(A) M. Pyda, B. V. Lebedev, M. Bartkoviak, and J. Grebowicz, Measurement and Computation of Heat Capacities of Benzene, *p*-Oligophenyls, and Poly-*p*-phenylene by the Advanced THermal Analysis, ATHAS; (B) *M. Pyda, W. Chen, and A. Habenschuss, Study of the Mesophases of PEIM by Thermal Analysis, Invited Lecture and poster at the IUPAC Symposium on Polymer Morphology and Electrical Properties, in Łódź, Poland, July 4–7.

*M. Pyda, and M. Bartkowiak, The ATHAS Data Bank. Lecture at the Institute of Physics, A. Mickiewicz University, Poznan, Poland, July 11.

*M. Pyda W. Chen, and A. Habenschuss. Study of the Mesophases of PEIM by Thermal Analysis, Lecture at the Institute of Physics, Technical University of Poznan, in Poznan, Poland, July 12.

*Y. Fu, Full Pattern X-ray analysis of Polymer Fibers. Invited Lecture at the Fibers Gordon Conference in New London, NH, July 9–14.

(A) The Structure and Defects of Fibers with Multiple Phase Structures and Their Correlation to Properties and Processing; (B) A. Habenschuss, W. Chen, M. Pyda, M. Varma, and H. S. Aldrich, X-ray Powder Diffraction Study of a

Symmetric Neopolyol Ester, Invited lecture and poster at the 1995 Denver X-ray Conference in Colorado Springs, July 31–August 4.

1995 cont. *M. Pyda, The ATHAS Scheme on Measurement and Computation of Heat Capacities of Solids, Liquids, and Mesophases of Linear Macromolecules and Small Molecules. Invited Lecture at the Technical University Gdansk, Faculty of Chemistry, Gdansk, Poland, August, 11,1995.

*M. Pyda, The ATHAS Scheme on Measurement and Computation of Heat Capacities of Polymers. Invited Lecture at the Inst. of Nuclear Chemistry and Technology, Warsaw, Poland, August, 12 and 13.

(A) Reversible and Irreversible Thermodynamics, Kinetics, and Measurement of Mass; (B) Measurement of Temperature and Heat. (C) Glass Transition. (D) Melting and Disordering Transition Four Tutorial Lectures; (E) Modulated Differential Scanning Calorimetry; Plenary lecture, and (F) Ge Zhang, B. V. Lebedev and J.-Y. Zhang, Heat capacities of Poly(amino acid)s and Proteins; (G) A. Boller, How to Approach Temperature Modulated DSC. (H) M. Varma-Nair, M. Pyda, W. Chen, A. Habenschuss, and H. S. Aldrich, Analysis of Disorder and Mobility is Symmetric Neopolyol Ester; Three Contributed Lectures at the 24th North American Thermal Analysis Society Conference, NATAS, in San Francisco, Sept. 10–13.

Travel to Australia to lecture at the 10th Royal Australian Chemical Institute Meeting. (Travel with Heidel, see pages 9-59–62 and Figures 62–65 of Chapter 9.)

The Meeting started with an invited lecture on Introduction to Modulated Differential Scanning Calorimetry, followed by a lecture at the Workshop on Thermal Analys: The Advanced Thermal Analysis System, ATHAS. Next, a contributed lecture on Multiple Phase Description of Polymers was given at the General Meeting, followed again by two lectures at the Workshop on Thermal Analysis: (A) First Order Transitions in Polymers; (B) Glass Transitions in Polymers. Only then was the Plenary Lecture scheduled: Learning How to Link Molecular Motion in Polymers to Thermal Analysis. All six contributions were given in sequence at the 10th Royal Australian Chemical Institute Meeting, Adelaide, South Australia, Sept. 27–Oct. 2.

Thermal Analysis of Nonequilibrium Polymers. Invited lecture at the Research Lab of Eastman Chemicals, Kingsport, TN on Nov. 1.

Modulated Differential Scanning Calorimetry. Weissberger-Williams lecture at Eastman Kodak, Rochester, NY on Nov. 15.

*A. Boller, Modulated DSC, Workshop at TA Instruments, New Castle, DE, October 31, 1995

*Y. Fu, Full Pattern Analysis of Fibers by X-ray Diffraction. Workshop at the Shell Development Co. Houston, TX, December 4–5.

*A. Boller, Introduction to Thermal Analysis. Invited lecture at Invequimica S. A., Medellin, Columbia, December 20.

1996 *Wei Chen, Study of Molecular Motion of a Poly(ester imide) by Solid State 13C NMR. Poster at the 37th Experimental Nuclear Magnetic Resonance Conference (ENR), Pacific Grove, CA, March 17–22.

(A) Frequency Dependence of the Glass Transition of Polymers by Temperature-modulated DSC; (B) Ge Zhang, Heat Capacity of Solid State Globular Proteins; (C) R. Festag, S. D. Alexandratos, and K. D. Cook, Separation and Characterization of Single-chain Polymer Particles. Three contributed lectures at the Am. Physical Society Meeting in St. Louis, March 17–22.

(A) Thermodynamic Functions and Modulated Calorimetry; (B) Phase Transitions. Two tutorials at the 20th Conference on Thermal Analysis in Polymer Research and Production, Park Ridge, NJ, April 15–17.

Temperature-modulated Measurements of the Apparent, Frequency-dependent Heat Capacity in the Glass-transition Region. Invited Lecture at the Midwest Thermal Analysis Forum, Minneapolis, MN, April 26.

Temperature-modulated Measurements of the Apparent, Frequency-dependent Heat Capacity in the Glass-transition Region. Lecture at Virginia Polytechnic Institute, Blacksburg, VA, May, 9.

*A. Boller, Temperature-modulated DSC, Lecture at the Ohio Regional Thermal Analysis Symposium, Columbus, OH, May 15.

Travel to Russia, Germany, and England (Accompanied by Heidel.)

Metastable Mesophases. Invited lecture at the 2nd International Symposium on Molecular Order and Mobility in Polymer Systems in St. Petersburg, Russia, May 21–24. [See also the mention in Appendix B, page B-23.]

Conformational Disorder in Amphiphilic and Thermotropic Smectic Phases—They May have a Common Border. Lecture at the Sonderforschungsbereich of the University of Freiburg, Freiburg,Germany, May 30.

Die Grundlagen der Temperature-Modulierten Wärmeflußdifferentialkalorimetrie. Lecture, Hüttenkolloquium in Neustadt, Schwarzwald, Germany, May, 31.

Reversible und Irreversible Phasenumwandlungen in Mesophasen und Kristallen. Invited Lecture in the Physics Colloquium Series of the University of Rostock, Germany, June 3.

(A) Specific Heat Capacity Determination by Modulated DSC and its Separation from Transition Effects (see publication 427 in Appendix A), invited lecture; and (B) A. Boller, Asymmetry of the Temperature Calibration in TMDSC, poster. Both at the Fourth Lähnwitz Seminar on the topic of 'Temperature-modulated Calorimetry,' held in the "Schloßpark Hotel Krugsdorf" near Pasewalk, Germany, June 4–7. (See page 9-52.)

*R. Festag, S. D. Alexandratos, K. D. Cook, D. C. Joy, P. J. Phillips, Synthesis and Characterization of Single Macromolecules: Mechanistic Studies of Crystallization and Segregation. Poster at the Microgravity Science Conference, Huntsville, AL, June 10–11.

(A) Fundamental Aspects of Temperature-modulated Differential Scanning Calorimetry of Polymers; (B) The Frequency-dependent Heat Capacity in

the Glass-transition Region. Tutorials at the two-day Thermal Methods Course at the University of Surrey, in Guildford, England, June, 10–12.

1996 cont. *A. Boller, Introduction to Temperature-modulated Calorimetry, lecture at Mettler-Toledo, Switzerland, June 13–14.

*Ge Zhang, Heat Capacity of Solid State Proteins by Thermal Analysis. Contributed lecture at the 51st Calorimetry Conference, Vancouver, Canada, August 3–10.

A major effort was made by the ATHAS Group and many of my former students to attend the 11th ICTAC in Philadelphia, PA, in connection with my receiving the TAI-ICTAC Award, and to participate in my 65th birthday celebration
(For details see Chapter 9 pages 9-52–54 and Figures 51–54.)

The meeting began with *two tutorials* on August 11 and 12: (A) The Basis of Thermal Analysis; (B) Thermal Analysis of the Polymer Phase Transitions. This was followed by the *Award Lecture*: (C) Learning about Calorimetry. Two *invited lectures* were given within the workshop "Two Phases or Three?": (D) Modeling Temperature-modulated DSC for the Measurement of Heat Capacity through the Glass Transition Region; (E) Detection of Multiple Nanophases by DSC. Three *contributed lectures* were given by my students: (F) A. Boller, Cell Asymmetry in DSC and TMDSC; (G) M. Pyda, Heat Capacities and Thermodynamic Properties of Benzene, *p*-Oligophenyls, and Poly-*p*-phenylene by Thermal Analysis; (H) A. Boller, Polyethylene Fibers, Multiple Melting Peaks in High Molar Mass, Gel-spun Polyethylene. The *Student Award* was presented to Ge Zhang. He gave the lecture (I) Heat Capacity of Solid State Proteins by Thermal Analysis. Finally, a *poster* was presented by I. Okazaki: (J) Modulated DSC in the Glass Transition Region. All at the 11th ICTAC/NATAS Meeting in Philadelphia, PA, August 11–16.

Seventh trip to Japan, Meeting of the IUPAC in Osaka
(Travelling with Heidel, see pages 9-56–57 and Figure 59 in Chapter 9.)

(A) The Kinetics of the Glass Transition as Described by the Hole Theory and Measured by TMDSC. (B) Temperature-modulated Heat-flux Calorimetry, A Theoretically Sound Method to Measure Total and Reversible Heat Capacity under Steady State Conditions. Two invited lectures at the Chemical Thermodynamics Meeting of the IUPAC in Osaka, Japan, held from August 25 to 30.

(A) Mesophases and their Glasses. (B) Rigid-amorphous and Mobile-oriented Phases in Bulk, Fibers, and Film. Two lectures given at the Toray Industries Laboratory, Otsu, Japan, September 2.

Heat Capacities by Standard and Temperature-modulated DSC for Polymers and Proteins. Lecture given at Nagoya University, Nagoya, Japan, September 4.

Temperature-modulated Measurements of the Apparent, Frequency-dependent Heat Capacity in the Glass-transition Region. Tutorial at the JIMA Instrument

Exhibition in Tokyo, Japan (which was supported by TA Instruments, Japan), September 5–6.

1996 cont. Modulated Calorimetry, A New Method to Study Reversible and Irreversible Processes. Seminar at Franklin and Marshall College, Harrisburg, PA, September 26.

Modulated DSC of Nonequilibrium Solids. Seminar at Albemarle Research Center, Baton Rouge, LA, October 22.

1997 Analysis of Polymers by Temperature-modulated Calorimetry, seminar at Cargill Research Laboratories in Wayzata, MN, Feb.18.

(A) Melting of Locally Reversible and Irreversible Crystallinity with TMC, a contributed lecture, and (B) A. Boller, Thermodynamic Properties of Gel-spun Ultra-high Molar-mass Polyethylene Fibers, a poster at the American Physical Society Meeting in Kansas City, MO, March 17–21.

Metastable Microphases and Nanophases in Polymers. Invited lecture at the Spring Meeting of the Materials Research Society in San Francisco, CA March 30–April 4.

Temperature-modulated Scanning Heat-Flux Calorimetry. Lecture at Alza Co., Palo Alto, CA, April 4.

Temperature-modulated Calorimetry of the Frequency Dependence of the Glass Transition of Poly(ethylene terephthalate). Invited Lecture at the 213th American Chemical Society Meeting in San Francisco, San Francisco, CA, April, 13–17.

The Advanced THermal Analysis System for Linear Macromolecules, Part A: Thermodynamic Functions and Modulated Calorimetry; Part B: Phase Transitions. Lectures given at the 21st Annual Course on Thermal Analysis of the Polytechnic Polymer Research Institute, in Newark, NJ, May 5–7.

*A.Boller, Thermodynamic Properties of Gel-spun Polyethylene Fibers, Colloquium at the ETH, Zürich, Switzerland, May, 16.

*A. Boller, Temperature-modulated DSC, Lecture and discussion at Mettler-Toledo AG, Greifensee, Switzerland, May, 15.

Travel to Germany and Spain (Accompanied by Heidel.)

Die Analyse des Glasumwandlungs- und Schmelzbereichs mit temperatur-modulierter Kalorimetrie (TMC). Lecture at the Polymer Research Division, Polymer and Solid State Physics, BASF, Ludwigshafen, Germany, July 4.

Evaluation of the Kinetics of the Glass Transition of PET as a Function of Crystallization History by Temperature-modulated Calorimetry with Minimal Instrument Lag. Invited lecture at the Third International Discussion Meeting on Relaxations in Complex Systems. Vigo, Spain, July 6–11.

*M. Pyda, Heat Capacity of Poly(trimethyl terephthalate) in the Melting Region by TMDSC. Lecture at the Calorimetry Conference (CALCON'97), Asilomar Conference Center, Pacific Grove, CA, during August 3–8.

1997 cont. Nanophase Separation in Smectic Liquid Crystals. Invited Lecture at the fourth International Symposium on Polymers for Advanced Technologies. Leipzig, Germany, August 31–September 4.

A Tutorial on the Basis of Thermal Analysis. Tutorial in connection with the 25th NATAS Conference in McLean, VA, Sept. 5–6.

(A) Melting by Temperature-modulated Calorimetry; (B) First Order Transitions by TMDSC; (C) W. Chen, M. Dadmun, G. Zhang, A. Boller, Isotropization on Nematic Liquid Crystals by TMDSC; (D) G. Zhang, Heat Capacities of Solid Proteins by Thermal Analysis; (E) M. Pyda, A. Boller, J. Grebowicz, H. Chuah, Heat Capacity of Poly(trimethylene terephthalate). Five lectures and one poster: (I) Jeongihm Pak, Sample-mass Effect to Temperature Calibration of Indium. All presented at the 25th NATAS Conference in McLean, VA, Sept. 7–9.

A Temperature-modulated DSC Study of the Melting of Polymers. Invited Lecture at the TA Instruments Seminar at McLean, VA. Sept. 10.

(A) A Temperature-modulated DSC Study of the Melting of Polymers, and (B) The Advanced Thermal Analysis Systen (ATHAS) for the Analysis of Polymers and Discussion of the Thermal Properties of Poly-*p*-dixoxanone and Poly(trimethylene terephthalate). Two lectures at the Shell Development Center, Westhollow, TX, Oct. 20.

Temperature-modulated Calorimetry of Polymers. Invited lecture at William and Mary College, Williamsburg, VA, November 7.

Travel to the Netherlands and Belgium (Together with Heidel.)

New Tools to Analyze Polymer Crystallization and Morphology. Lecture at Eindhoven University of Technology, Eindhoven, The Netherlands, Nov. 29.

New Ideas and Analyses of the Structure of Polymers. Lecture at the research laboratory of DSM, Geleen, Netherlands, December 1.

New Ideas and Analyses of the Structure of Polymers. Lecture at the Catholic University of Leuven, Leuven, Belgium, December, 2.

Three lectures in the Symposium on "Crystallization and Morphology of Polymers." I. Crystallization and Melting Kinetics. II. Crystal Structure of Polymers. III. Crystal Morphology. Leuven, Belgium, December 3–4.

Temperature-modulated DSC of Polymers. Lecture at the Vrije Universiteit, Brussels, Belgium, December 4.

1998 Is Complex Heat Capacity a Useful Output of Temperature-modulated Calorimetry? Invited Lecture at the 215th Americal Chemical Society Meeting (Division of Polymeric Materials), Dallas TX, March 29–April 2.

*M. Pyda and M. Bartkowiak, Conformational Heat Capacity of Interacting Systems of Polymers and Small Molecules, Contributed lecture at the American Physical Society Meeting in Los Angeles, CA, March 16–20.

1998 cont. Part A: The Advanced THermal Analysis System for Linear Macromolecules, Part B: Thermodynamic Functions and Modulated Calorimetry; Part C: Phase Transitions; and a lecture on Temperature-modulated Calorimetry. Three lectures at the 22nd Annual Course on Thermal Analysis of the Polytechnic Polymer Research Institute, in Newark, NJ, April 20–22.

(A) *M. Pyda, Temperature-modulated Differential Scanning Calorimery of Poly(trimethylene terephthalate) and Paraffins; (B) *W. Chen, Detailed Analysis of Isotropizatiopn of Small and Macromolecular Liquid Crystals by Temperature-modulated DSC; two poster at the First ICI Northamerican Science and Technology Conference in Strongsville, OH, April 20–22.

Application of the Advanced THermal Analysis System (ATHAS) to DSC and Temperature-modulated DSC of Polymers. Keynote Lecture at the Soc. Plastics Engineers ANTEC'98 Meeting, Atlanta, April 26–30.

(A) Liquid Crystals and Nanophases in Polymeric Material; (B) Temperature-modulated Differential Scanning Calorimetry. Invited lecture and tutorial at the RayChem Research Laboratory, Menlo Park, CA, May 13.

(A) Liquid Crystals; (B) Heat Capacity of Solid Stater Proteins; (C) Application of Temperature-modulated Calorimetry. Mini lectures, invited lecture, and tutorial at "inhale" Therapeutic Systems, San Carlos, CA, May 13–14.

Travel to the 5th Lähnwitz Seminar in Kühlungsborn (Accompanied by Heidel and attended after a vacation trip to the Norwegian Fjords, described on pages 9-73–77.)

(A) Temperature-modulated Differential Scanning Calorimetry of Reversible and Irreversible First-order Transitions (see publication 476 in Appendix A). Opening Lecture at the Lähnwitz Seminar on 'Investigation of Phase Transitions by Temperature-modulated Calorimetry;' and (B) M. Pyda, Temperature-modulated Differential Scanning Calotimetry of Poly(trimethylene terephthalate) and Paraffins in the Melting/Crystallization Region (see also publication 452 in Appendix A); poster, both at the 5th Lähnwitz Seminar in Kühlungsborn, Germany, June 7–12.

(A) *M. Pyda, Heat Capacity, First-order and Glass Transitions Analyzed by Temperature-modulated Calorimetry, and (B) *M. Pyda and J. Grebowicz. Heat Capacity of Poly[carbonyl(ethylene-*co*-propylene)]. Two contributed lectures at the 7th European Symposium on Thermal Analysis and Calorimetry. Balatonfüred, Hungary, August 30–September 4.

*M. Pyda. The Advanced THermal Analysis of Macromolecules and Small Molecules by DSC and TMDSC. Seminar at the Dept. of Physics of the A. Mickiewicz University of Poznan, Poland, September 8.

*M. Pyda. (A) Temperature-modulated Differential Scanning Calorimetry of poly(trimethylene terephthalate) in the Melting/Crystallization Region. (B) Computation of the Capacity of Polymers in the Liquid State. Seminar and group discussion at the Polytechnic of Poznan, Poland, September 10.

1998 cont. The Basis of Thermal Analysis and Temperature-modulated Calorimetry of Materials. Three tutorial Lectures at the NATAS Thermal Analysis Short Course, Cleveland, OH, September 11–12.

(A) Heat Capacity; (B) I. Moon and R. Androsch, Optimum Conditions for Accurate Heat Capacity Measurements in Temperature-modulated Differential Scanning Calorimetry; (C) W. Chen and A. Toda, Analysis of transitions of Liquid Crystals and Conformationally Disordered Crystals by Temperature–Modulated DSC Latent Heats and TMDSC; (D) J. Pak, A. Boller, I. Moon, and M. Pyda, Thermal Analysis of Paraffins by Calorimetry. (E) Y. K. Kwon, M. Pyda, and W. Chen, Thermal Properties of Poly(ester-imide)s with $C_{12}H_{24}$ and $C_{22}H_{44}$ Alkyl Groups; (F) R. Androsch, Melting and Crystallization of Poly(ethylene-*co*-octene) measured by Modulated DSC and Temperature-resolved X-ray Diffraction; (G) M. Pyda, Computation of Liquid Heat Capacities of Polymers; Seven contributed Lectures and (H) M. Pyda, Analysis of Lissajous Figures from TMDSC of Melting and Crystallization of Polymers and Small Molecules; (I) M. L. DiLorenzo, G. Zhang, and M. Pyda, Heat Capacities of Polypeptides by Thermal Analysis, two posters, all given at the 26th NATAS Meeting in Cleveland, OH, on September 13–15, 1998.

Analysis of Polymers by AFM and Microcalorimetry. Invited Lecture at the TA-Instruments Seminar on Micro-thermal Analysis and MDSC for Pharmaceutical Applications. Cleveland, OH, September 16–17.

(A) M. Pyda, Temperature-modulated DSC of Poly(trimethylene terephthalate) and Paraffins in the Melting/Crystallization Region; (B). W. Chen, Study of Polyethylene Fiber by Solid State 13C NMR Spectroscopy. Two posters at the UTK Departmental Research Symposium, Knoxville, September 24–25.

New Ideas and Analyses of Polymers. Recruiting Seminar at The Appalachian State University, Boon, NC, October 23.

Introduction to Temperature-modulated Differential Thermal Analysis, Recruiting Seminar at The University of Western Florida, Pensacola, FL, November 6.

1999 A series of four Lectures on Differential Scanning Calorimetry and Temperature-modulated Differential Scanning Calorimetry were given at the Dept. of Chemistry of the University of Tennessee, Knoxville, TN, Feb. 2–March 16.

Temperature-modulated Differential Scanning Calorimetry of Reversible and Irreversible First Order Phase Transitions. Invited lecture at the local American Chemical Society Section at Raleigh, NC, March 11.

(A) Reversible and Irreversible First-order Phase Transitions Analyzed by Temperature-modulated Calorimetry; (B) M. Pyda, The Role of Degeneracy in the Conformational Contribution to the Liquid Heat Capacity of Branched Polymers; (C) R. Androsch, J. Blackwell, S. N. Chvalun, Wide-angle and Small-angle X-ray Analysis of Poly(ethylene-*co*-octene); (D) Y.-K. Kwon, The Effect of Strain on Gel-spun, Ultrahigh Molar Mass Polyethylene Fibers; (E) W. Chen, The Study of the Crystallization Kinetics of Main-chain Liquid-crystal Polymers by Using Temperature-modulated Calorimetry; five

contributed papers and (F) I. K. Moon, R. Androsch, W. Chen, Micro-thermal Analysis of Macromolecules; one poster at the American Physical Society Centennial Meeting, Atlanta, GA. March 20–26.

1999 cont. Using Thermal Analysis for Predicting Lifetimes. An invited lecture at the 22nd Aging, Compatibility and Stockpile Stewardship Conference, held at ORNL, Oak Ridge, April 27–29.

Temperature-modulated Differential Scanning Calorimetry of Reversible and Irreversible First-order Transitions. Invited Lecture at the research laboratories of RayChem, Menlo Park, CA, May 14.

Reversible and Irreversible First Order Phase Transitions Analyzed by Temperature-modulated Calorimetry. Invited lecture at the Central Research Laboratory of the DuPont Co., Wilmington, DE, August 10.

(A) *Marek Pyda. Heat Capacity by Multi-frequency Sawtooth Modulation, (B) *Marek Pyda. Computation of Liquid Heat Capacities of Polymers and Small Molecules. Two Presentation at the 57th Calorimetry Conference (Calcon'99) in Talahassee, FL, August 15–20.

Analysis of the Nanophase Structure of Semicrystalline Polymers with Atomic Force Microscopy (AFM), microcalorimetry (MC), and Temperature-modulated Calorimetry. Invited Lecture at the Fall Meeting of the American Chemical Society, August 22–27, New Orleans.

*L. Di Lorenzo, Temperature-modulated Calorimetry of the Crystallization of Polymers Analyzed by Measurements and Model Calculations, contributed lecture at the 14th Convegno Italiano di Scienza e Technologia delle Macromolecole, at the University of Salerno, Italy, September 13–16.

*M. L. DiLorenzo, Miscibility, Crystallization and Melting Behavior of Poly(amid-ether) Multiblock Copolymers, poster at the Meeting of the Consiglio Nazionale Delle Richerche on "I Materiali Polymerici per il 21° Secolo." Napoli, Italy, September 18–20.

A series of one plenary lecture, five contributed lectures and one poster were scheduled to be given at the 27th Annual North American Thermal Analysis Society Meeting in Savannah, GA, September 19–22. Hurricane Floyd caused a cancellation of the Meeting and the various presentations are recycled as lectures in other locations. Despite the lost Meeting, the Proceedings have been published. (See Appendix A, publications 450, 493, 492a, 491a, 490a, 486a, 485b, and 448a.)

The Basis of Thermal Analysis, three-hour tutorial at the Thermal Analysis Short Course of the North American Thermal Analysis Society in Saint Louis, MO, September 23–24.

Thermal Analysis in the Glass Transition Region, 1½ hour Tutorial at the Thermal Analysis Short Course of the North American Thermal Analysis Society in Saint Louis, MO, September 23–24.

Reversible and Irreversible Melting. Invited Lecture at the Workshop of TA Instruments, Inc. in Saint Louis, MO, September 25–26.

Analysis of Nanophases of Polymers by Atomic Force Microscopy, Micro-calorimetry, and Temperature–Modulated Calorimetry. Invited Lecture at

the Microthermal Analysis Seminar of TA Instruments, Inc. in Saint Louis, MO, September 27.

1999 cont. Reversible and Irreversible Melting by Temperature-modulated Differential Scanning Calorimetry. Invited Lecture at the Research Laboratory of MMM, Minneapolis, MN, November 8.

2000 Glass and Melting Transitions of the Mesophase in Gel-spun, Ultra-high-molar-mass Polyethylene Fibers. Lecture at the American Physical Society March Meeting, Minneapolis, MN, March 20–24.

Polypropylene, Discussion at the Research Laboratory of MMM, Minneapolis, MN, March 21.

(A) M. Pyda, Conformational Contribution to the Heat Capacity of Starch and Starch-Water; (B) R. Androsch, Reversible Crystallization and Melting of Poly(ethylene-*co*-octene); (C) J. Pak, Melting and Crystallization of Paraffins by Calorimetry. Three lectures and one poster: (D) R. Androsch, A Study of the Annealing of Poly(ethylene-*co*-octene) by Standard and Modulated DSC. All presented at the American Physical Society, March Meeting in Minneapolis, MN, March 20–24.

Thermal Properties and Nanophase Structure of Poly(trimethylene terephthalate). Invited Lecture at the American Chemical Society Meeting, ACS Award for Team Innovation in honor of the Shell Corterra Team, San Francisco, given in March 26–30.

The Present and Future Applications of Microcalorimetry. Invited Lecture at the Second International Meeting on Microcalorimetry at the University of Western Kentucky in Bowling Green, KY, May 7–8.

(A) Temperature-modulated Calorimetry of Polymers with Single- and Multiple-frequency Temperature Modulation to determine C_p and Reversible and Irreversible Transition Parameters. Invited lecture at the ASTM Symposium on Materials Characterization by Dynamic and Modulated Thermal Analysis Techniques; and (B) The Temperature Distribution in a Temperature-modulated DSC as Determined by Infrared Thermography, a lecture to introduce a panel discussion. All in Toronto, Canada, May, 2–16.

Travel to Gargnano, Italy and the 6th Lähnwitz Seminar in Germany
(The trip was taken together with Heidel.)

Irreversible and Locally Reversible Melting and Crystallization Studied by Temperature-modulated Calorimetry. Invited Lecture at the Europolymer Conference 2000 (EUPOC 2000) in Gargnano, Italy, May 28–June 1.

(A) The Measurement of Heat Capacity at Time-scales from Pico to Megaseconds, Opening lecture at the 6th Lähnwitz Seminar on 'Frequency and Time Dependent Heat Capacity' (see publication 504 in Appendix A); and (B) M. Pyda, Heat Capacity by Multi-frequency Saw-tooth Modulation. Poster (see also publication 475 in Appendix A), both at the 6th Lähnwitz Seminar in Kühlungsborn, Germany, June 12–18.

2000 cont. *M. Pyda, Thermal Properties of PTT by Calorimetry. Invited Lecture at the Martin Luther University in Halle, Germany, June 26.

*M. Pyda, Thermal Properties of Polymers by Calorimetry. Invited lecture at the Institute of Physics of the University of A. Mickiewicz in Poznan, Poland, given onJune 29.

(A) *M. Pyda, Heat Capacity Spectroscopy of Polymers; (B) *M. Pyda, Thermal Properties of Poly(ethylene terephthalate) by Temperature-modulated Differential Scanning Calorimetry. (A) lecture and (B) poster at the 38th Macromolecular Symposium in Warsaw, Poland, July 9–14.

*M. Pyda, Heat Capacity by Multifrequency Sawtooth Modulation. Invited lecture at the Institute of Physics of the University of A. Mickiewicz in Poznan, Poland, July 18.

Travel to the 12th ICTAC in Denmark (Together with Heidel.)

Modulation of the Sample Temperature in DSC with Multiple Frequencies. Lecture at the 12th ICTAC in Copenhagen, Denmark, August 14–18.

Teaching of "Thermal Analysis of Materials." Presentation at the Workshop of the ICTAC Education Committee at the 12th ICTAC in Copenhagen, Denmark, August 14–18.

Second trip to China (With Heidel, see Chapter 9, pages 62–66 and Figures 66–67.)

Influence of Dynamics and Structure on the Thermodynamic Properties and Transitions of Polymers. Two-hour invited lecture and discussion at Fudan University, Shanghai, China, September 7.

Influence of Dynamics and Structure on the Thermodynamic Properties and Transitions of Polymers. Invited lecture at the International Symposium on Polymer Physics, PP'2000, Huangshan, China, September 13–17.

(A) High Quality Heat Capacity Measurements at Different Frequencies of Temperature Modulation; (B) J. Pak, Melting and Crystallization of Low Molecular Weight Polyethylene by Calorimetry; (C) A. Kamasa, Characterization of the Ceramic Coating of Iron with TiN by Temperature-modulated Thermomagnetometry; (D) A. Kamasa, Multi-frequency Heat Capacity Measurement by Different Types of Temperature Modulation; (E) M. Pyda, Reversible and Irreversible Apparent Heat Capacities of Poly(carbonyl-*alt*-ethylene-*co*-propylene) by Temperature-modulated Differential Scanning Calorimetry; five Lectures at the 28th NATAS Conference in Orlando, FL, October 4–6.

2001 Differential Thermal Analysis of Materials. Presentation at the local Society of Plastic Engineers (SPE) Section in Knoxville, TN on January 25.

The Importance of the Measurement of Heat Capacity for Quantitative DSC and TMDSC. Plenary Lecture at the TA Tnstruments Technology Seminar, Newark, DE, January 28–30.

2001 cont. (A) Reversibility of Melting of Polyethylene of Different Mass; (B) Marek Pyda, Conformational Contribution to the Heat Capacity of the Interacting System of Carbohydrate Polymer and Water; two contributed lecture and one poster, (C) J. Pak, M. Pyda, Critical Chain Length for the Need of Supercooling of Extended-chain Crystals of Oligomers by Calorimetry; given at the American Physical Society Meeting, Seattle, WA, March 12–16.

(A) The Importance of the Measurement of Heat Capacity for Quantitative DSC and TMDSC. (B) Marek Pyda, The Calorimetry of Polylactide. Two lectures at Cargill Dow Polymers LLC, Minnetonka, MN, given on May 3.

Travel to Belgium (Accompanied by Heidel.)

Differential Thermal Analysis of Materials. Plenary Lecture at the General Meeting of the Belgian Polymer Group in Sunparks, Mol, Belgium, May 16–17.

2001–2006 Knoxville, TN

Retirement on June 1

(Maintaining the laboratories at UTK and ORNL with support by the Polymer Program of NSF).

2001 No change in Residence.

2001, cont. *Marek Pyda, New Advances in Data Analysis and Interpretation of Biopolymer-Water Systems. Poster at the 2001 Biocalorimetry Conference, Philadelphia, PA, July 26–28.

*Marek Pyda, Analysis of the Residual Entropy of Amorphous Polyethylene at 0 K Derived from Heat Capacity. Oral Presentation at the 56th Calorimetry Conference, Colorado Springs, CO, July 29–August 3.

At the 29th NATAS Conference in St. Louis a two-day symposium in honor of my 70th birthday was arranged under the title 'The Solid State of Macromolecules.' Despite the short time after the September 11 terror attack (see page 3-36) almost all who had planned to attend the symposium, did so, and 21 papers were collected in a special issue of Thermochimica Acta, **396**, 1–232 (2003). See also pages 9-18 and 10-3.

(A) The Three Reversible Crystallization and Melting Processes of Semicrystalline Macromolecules; (B) Temperature-modulation with standard DSC; (C) M. L. Di Lorenzo, M. Pyda, Reversible Melting in Nanophase-separated Poly(oligomer amide-*block*-oligomer ether)s Probed by Temperature-modulated Calorimetry; (D) M. Pyda, Quantitative Thermal Analysis of Biomaterial-Water Systems; (E) P. Kamasa, A. Buzin, M. Pyda, The Use of Infra-red Light-modulated Temperature in DSC by Application of Pulse-width Modulation; (F) A. I. Buzin, P. Kamasa, M. Pyda, Application of Wollaston Wire Probes for Quantitative Thermal Analysis; six lectures and (G) J. Pak, M. Pyda, Critical Chain Length for the Growth of Crystals of Oligomers of Oxyethylene and Oxytetramethylene without Supercooling. A

Study with Temperature-modulated Calorimetry; (H) P. Kamasa, M. Pyda, A. Buzin, Frequency Dependence of the Heat Capacity of Polystyrene by Multi-frequency Infrared Temperature-modulated DSC in the Glass Transition Region; two posters presented at the 29th NATAS Conference in St.Louis, MO, September 24–26.

2001 cont. Temperature-modulated Differential Scanning Calorimetry of the Crystallization\Melting Equilibrium in Paraffins and Polyolefins. Invited lecture at the Polyolefins Workshop III, Sonoma, CA, October 7–10.

Differential Thermal Analysis. Invited Lecture at Pfizer, Groton, CT, December 3.

2002 Mesophases. Invited Lecture at Pfizer, Groton, CT, February 8.

The Glass Transition as Seen by Thermal Analysis. Tutorial at the American Physical Society Short Course on the Glass Transition, March Meeting in Indianapolis, IN, March 16–22.

(A) J. Pak, Reversible Melting of UHMMPE and PE Extended-chain Crystals Detected by Temperature-modulated Calorimetry; (B) M. Pyda and R. C. Bopp, Heat Capacity of Poly(L-lactic acid). (C) Analysis of the Residual Entropy of Amorphous Polyethylene. Three contributed lectures and (D) E. V. Kosyreva, A. I. Buzin, and M. Pyda, An Integrated Approach to the ATHAS Data Bank; four contibuted lectures and (E) A. I. Buzin, M. Pyda, K. Matyaszewski, Calorimetric Study of Gradient Block-copolymers of Poly(butylacrylate) and Poly(methylmethacrylate); two posters given at the Am. Physical Society March Meeting in Indianapolis, IN, March 16–22.

*M. Pyda, Charakteryzacja Polimerów za Pomocą Kalorymetrii. Invited Lecture at the Polish Academy of Sciences, Łòdź, Poland, April 10.

*M. Pyda, Własności Termodynamiczne Polimeròw i Małych Cząsteczek Badane Metodami Kalorimetrii. Invited Lecture at the University of Poznan, Poznan, Poland, April 12.

*M. Pyda, Characterization of Fiber and Bulk Poly(trimethylene terephthalate) by Quantitative Thermal Analysis. Invited Lecture at the NaTex Texas and South West Thermal Analysis Forum on Timely Topics in Thermal Analysis, in San Antonio Texas, May 31–June 1.

3rd International Meeting on Polymer Crystallization, 8th trip to Japan (With Heidel.)

Reversible Crystallization and Melting of Polymers. Invited Lecture at the International Symposium on Polymer Crystallization in Mishima, Shizuoka, Japan, June 9–12. (See also the descriptions on pages 8-63 and 9-85 and the discussion on page 10-8–9).

Temperature-modulated DSC. Invited contribution to the Discussion Meeting on Structure Formation Mechanisms in Polymer Crystallization at the Uji Campus of the Kyoto University, June 14.

2002 cont. *Wenbing Hu, Simple Temperature-modulated DSC for Polymers, contributed lecture to the International Symposium on Polymer Physics in Qingdao, China, July 1–6.

*Wenbing Hu, A. Buzin, and J.-S. Lin, Annealing of Gel-spun Fibers before Significant Annealing, IUPAC World Polymer Congress, 39th International Symposium on Macromolecules in Beijing, China, July 7–12.

Travel to the 7th Lähnwitz Seminar, Germany (Accompanied by Heidel.)

(A) Calorimetry of Polymer Nanophases of Crystals, Mesophases, Glasses and Liquids. Invited Lecture, 7th Lähnwitz Seminar on 'Thermodynamics and Calorimetry of Small Systems' (see publication 530 in Appendix A), Rostock (part of the Conference the IUPAC's 17th ICCT). (B) M. Pyda, 'Analysis of the Residual Entropy of Amorphous Polyethylene at 0 Kelvin Derived from Heat Capacity'; (C) M. Pyda, Glass Transition and Heat Capacity of Biomaterial-Water Systems; three lectures and (D) J. Pak, M. Pyda, 'Rigid Amorphous Fraction in Poly(phenylene oxide) Detected by Temperature-modulated Calorimetry,' a poster at the 17th IUPAC Conf. on 'Chemical Thermodynamics' in Rostock, Germany, July 28–Aug. 02.

(A) *M. Pyda, A. Buzin, R. C. Bopp, Morphology of Poly(lactic acid) by AFM and Calorimetry; (B) *J. Pak, M. Pydal, Rigid-amorphous Fraction in Poly(phenylene oxide) Detected by Temperature-modulated Calorimetry; two lectures at the 30th NATAS Conf. in Pittsburgh, PA, Sept. 23–25.

The Solid State of Semicrystalline Macromolecules, the First Nanophase Material for Industry—Temperature-modulated Calorimetry, the First Experimental Method to Study the Phase-behavior of Polymeric Nanophases, Plenary Lecture at the 10th International Conference "Polymeric Materials 2002" on the occasion of the 500 year anniversary of the University of Halle, Halle, Germany Sept. 25–28. (See also publications 507 in Appendix A.)

*M. L. Di Lorenzo, Analysis of Polymer Melting by Temperature-modulated Calorimetry. Effect of Latent Heat Contributions to the Reversing Heat Capacity. Invited Lecture at the XXIVth National Meeting of Calorimetry, "Thermal Analysis and Chemical Thermodynamics," Catania, Italy, December 15–18.

2003 (A) Evidence for Coupling and Decoupling of Parts of Macromolecules by Temperature-modulated Calorimetry; (B) M. Pyda, R.C. Bopp, Reversible and Irreversible Heat Capacity of Poly(lactic acid) Analyzed by Temperature-modulated Differential Scanning Calorimetry. Two contributed lectures and (C) M. Pyda, J. Pak, and B.W., Characterization of Fiber and Bulk of Poly(trimethylene terephthalate) by Quantitative Thermal Analysis; a poster at the Am. Phys. Soc. Meeting, Austin, TX, March 3–7.

*M. Pyda, E. Nowak-Pyda, Heat Capacity of Poly(lactic acid), Lecture at the 58th Calorimetry Conference (CALCON 2003), Hawaii, July 27–August 3.

2003 cont. The Tribulations and Successes on the Road from DSC to TMDSC in the 20th Century and the Prospects of Microcalorimetry in the 21st. Invited Feature Presentation at the Ohio Valley Thermal Analysis Society DSC Symposium and ASTM E37 Workshop at Western Kentucky University, Bowling Green, KY August 18–19. (See also Appendix B, page B-23.)

(A) Quantitative Temperature-modulated Calorimetry, invited lecture and (B) M. L. Di Lorenzo, Melting of Polymers by TMDSC: Influence of Irreversible Latent Heat to Reversing Heat Capacity; (C) M. Pyda, Reversing and Nonreversing Heat Capacity of Poly(lactic acid) in the Glass Transition Region by Temperature-modulated Differential Scanning Calorimetry; two contributed lectures at the 31st North American Thermal Analysis Society (NATAS) Conf. in Albuquerque, NM, September 22–24.

The Nanophase Structure of Semicrystalline Polymers and Its Influence on the Thermal and Mechanical Properties. Invited lecture, ACS Polymer Division, Meeting on: Advances in Polyolefins in Sonoma, CA, October 5–8.

*M.L. Di Lorenzo, Temperature-modulated DSC of Polymer Melting: Can Fourier Analysis Provide a Quantitative Separation of the Reversing and Total Heat Capacities? Invited lecture at the International Conference on: "Times of Polymers—TOP," held in Ischia, Napoli, Italy, October 2003.

Reversible and Irreversible Processes in the Temperature Range of Phase Transitions of Polyolefins and Paraffins. Invited Seminar at the Exxon Mobil Research and Engineering Co., Annandale NJ, November 10.

8th Pacific Polymer Conference (PPC8) in Thailand (With Heidel, see page 10-9.)

The Nanophase Structure of Semicrystalline Polymers and Its Influence on the Thermal and Mechanical Properties, Plenary Lecture at the 8th Pacific Polymer Conference (PPC8), Bangkok, Thailand, November 24–27.

2004 (A) Quantitative DSC and TMDSC, introductory lecture and (B) M. Pyda, Crystallinity of Polymers by Calorimetry and Quantitative Thermal Analysis; two contributions to a discussion at the TA Instruments 2004 Users Meeting and Symposium in San Antonio, TX, February 1–3.

Quantitative DSC and TMDSC. Invited Polymer Seminar at the Institute of Materials Science of the University of Connecticut, Storrs CT, March 5.

(A) Evidence for Coupling and Decoupling of Parts of Macromolecules by Temperature-modulated Calorimetry, invited lecture and (B) M. Pyda, E. Nowak-Pyda, Quantitative Thermal Analysis of Poly(butylene terephthalate) by Temperature-modulated Differential Scanning Calorimetry; a contributed lecture at the American Physical Society in Montreal, Canada, March 21–26.

*M. Pyda, Simultaneous Temperature-modulated Calorimetry of Polymers at low and high Frequencies to determine Heat Capacities. Invited Lecture at an ASTM Symposium in Philadelphia from May 24–25.

Travel to the 8th Lähnwitz Seminar in Warnemünde, Germany (Together with Heidel.)

2004 cont. (A) The Influence of the Surface on the Thermodynamics of Melting and Glass Transition of Films and Fibers. Invited lecture (see publ. 551 in Appendix A), and (B) M. Pyda, E. Nowak-Pyda, Thermal Characterization of Thin Films of Poly(lactic acid) by Calorimetry and AFM; poster (see also publication 531 in Appendix A), both at the 8th Lähnwitz Seminar on 'Thermodynamics and Calorimetry of Thin Films.' Warnemünde, June 6–10.

*M. Pyda, Thermodynamic Properties of Polymer Blends on Heat Capacity by Calorimetry. Invited lecture at the Technology University in Łódź, Poland, June 15.

Travel to give a Plenary Lecture in Cancún (Accompanied by Heidel. For prior trips to Cancún arranged as private tourist travel, see in Chapter 9, pages 9-66–67 and Figures 68–71 and also page C-65, below.)

The Nanophase Structure of Semicrystalline Polymers Investigated by Temperature-modulated Calorimetry. Plenary lecture at the XIIIth International Materials Research Congress in Cancún, Mexico, August 22–26.

(A) How to Use Thermal Analysis for the Six Dimensions of Polymer Characterization: 1. Synthesis, 2. Structure, 3. Processing, 4. History, 5. Properties, and 6. False Measurement, Short Course at the NATAS Conf. in Williamsburg, VA, Oct. 3. (B) The ATHAS Teaching Effort on Thermal Analysis of Polymeric Materials, Plenary Lecture and (C) Thermal Analysis of Polymeric Materials, Invited Seminar with Demonstrations at the NATAS Conference. (D) Fast and Super-fast DTA and Calorimetry; (E) The DSC and TMDSC of Poly(butylene terephthalate); (F) M. Pyda, E. Nowak-Pyda, Thermal Analysis and Morphology of Thin Films of Poly(lactic acid) by Calorimetry and AFM; invited lectures and (G) W Qiu, E. Nowak-Pyda J. Pak, M. Pyda, Effect of Pan Deformation on Heat-flow Rate; (H) M. Pyda, E. Nowak-Pyda, Thermal Analysis of Quenched Poly(butylene terephthalate) by Temperature-modulated Calorimetry; (I) Nowak-Pyda, M. Pyda, The Heat Capacity of Polyethylene Fibers Measured by Multi-frequency Temperature-modulated Calorimetry, three posters all of the last eight presentations were given at the NATAS Conf. in Williamsburg, VA, Oct. 4–6.

2005 (A) Effect of Confinement of the Amorphous Phase of Polymers in Semicrystalline Polymers; invited lecture and (B) M. Pyda, Relaxation Processes of the Amorphous and Semicrystalline Biodegradable Poly(lactic acid) by Temperature-modulated Calorimetry; a contributed lecture at the Division of Polymeric Materials: Science and Engineering of the American Chemical Society Meeting in San Diego, CA, March 13–17.

(A) (lecture given by M. Pyda:) Reversible Processes Between the Glass and Melting Transition of Poly(oxyethylene); (B) *M. Pyda, K., Van Durme, and B. Van Mele, Heat Capacity of Poly(vinylmethylether) in the Presence and

Absence of Water; (C) *R. Androsch, H.-J. Radusch, Reversible Melting of Extended-chain and Folded-chain Polymer Crystals; three contributed lectures at the American Physical Society, all presented in Los Angeles, CA, March 20–25 in my absence, due to a medical emergency.

2005 cont. *M. Pyda, Characterization of the Biodegradable Polymers by Modern Calorimetry and AFM. Invited Lecture at the University of Technology in Rzeszow, Poland, February 14.

Travel to the PPS21 in Leipzig, Germany (Together with Heidel.)

(A) Effect of Decoupling of Molecular Segments, Microscopic Stress-transfer, and Confinement of the Nanophases in Semicrystalline Polymers. Invited Keynote Lecture in Symposium No. 8; and (B) M. Pyda, E. Nowak-Pyda, Characterization of the Amorphous and Semicrystalline Biodegradable Poly(lactic acid) by Temperature-modulated Calorimetry; (C) R. Androsch, T. Lüpke , and A. Wutzler, Influence of Deformation on Irreversible and Reversible Crystallization of Poly(ethylene-*co*-1-octene); two contributed lectures also in the Symposium No. 8: "Morphology and Structure Development," at the Meeting of the Polymer Processing Society, PPS21, Leipzig, Germany, June 19–23. (See publ. 556, Appendix A and page 10-4.)

(A) The Contributions of MDSC to the Understanding of the Thermodynamics of Polymers. Invited lecture in the Symposium on Modulation Techniques/Fast Scan Thermal Analysis. (B) The Glass Transition of Polymer Crystals, two Invited Lectures, see publs. 562a,b and 563a,b in Appendix A. Furthermore two contributed lectures: (C) M. Pyda, E. Nowak-Pyda, Physical Aging of Amorphous Poly(lactic acid) by Temperature-modulated Calorimetry; (D) M. Pyda, K. Van Durme, B. Van Mele, Heat Capacity of Poly(vinyl Methyl Ether) in the Presence and Absence of Water. All presented at the 33rd NATAS Meeting in Universal City, CA, September 22–24.

The Decoupling of Polyolefin Chain-segments on Phase Boundaries and the Resulting Effects on Thermodynamic and Mechanical Properties. Invited Lecture to the ACS Division of Polymer Chemistry, Fourth Meeting on: Advances in Polyolefins, in Sonoma, CA, September 24–28.

*M. Pyda, E. Nowak-Pyda, Quantitative Thermal Analysis of Polymers by Modern Calorimetry, Part I. Invited Lecture at the University of Technology, Faculty of Physics in Rzeszow, Poland, October 27. (For Part II, see below.)

The Glass Transition of Liquids, Mesophases, and Crystals of Polymers and Small Molecules. Invited Lecture at the Department of Polymer Science at the University of Akron, Akron, OH, November 14–15.

*M. Pyda, Application of Ising-like Models to study of Conformation of Polymers and Polymer-Water Systems by Modern Calorimetry. Invited Lecture at the University of Technology, Fac. Phys. in Rzeszow, Poland, November 25.

2005 cont. *M. Pyda, Characterization of the Biodegradable Poly(lactic acid) by Modern Calorimetry and AFM. Invited Lecture at the University of Kassel in Kassel, Germany, November 28.

*M. Pyda, Quantitative Thermal Analysis of Polymers by Modern Calorimetry, Part II, invited lecture at the University of Technology, Faculty of Physics in Rzeszow, Poland, December 08. (For Part I, see above.)

2006 (A) Transitions of Polymers with Precise Oligomethylene Sequences; (B) M. Pyda, K. Van Durme, B. Van Mele, Heat Capacity of Liquid Poly(vinyl methyl ether) With and Without Water. Two contributed lectures, at the Am. Phys. Soc. Meeting in Baltimore, MD, March 12–17.

The Glass Transition as Key to Identify Phases by DSC and TMDSC. Invited Lecture at the Users Meeting of TAI, Inc. At Newport, RI, May 9–11.

Travel to the 9th Lähnwitz Seminar in Warnemünde, Germany (With Heidel.)

(A) 100 Years Research on Superheating and Supercooling. Invited Introductory Lecture (see publication 528 in Appendix A); and two posters: (B) M. Pyda, Heat Capacity of Liquid Poly(vinyl methyl ether) in the Absence and Presence of Water, and (C) M. Pyda, Melting and Crystallization of Poly(butylene terephthalate) (see publications 557 and 548 in Appendix A); 9th Lähnwitz Seminar on 'Transitions Far From Equilibrium—Superheating and Supercooling.' Rostock-Warnemünde, Germany, May 28–June 1.

2006– ***Knoxville, TN*, No change in Residence.**

Closing of the Laboratories on June 1

(Maintaining an office at UTK and continued teaching of the Computer Course).
(see Chapter 10 for details)
(To this date, approximately 1,200 presentations were given).

2006, cont. (A) The Calorimetry of Nanophases of Macromolecules. Invited lecture, and (B) M. Pyda, E. Nowak-Pyda, and K. Van Durme and B. Van Mele, Vrije Universiteit, Brussels, Belgium. Conformational Heat Capacity of Liquid Poly(Vinyl Methyl Ether) in the Absence and Presence of Water. Contributed lecture. Both at the THERMO International 2006, 16th Symposium on Thermophysical Properties in the Section "Semicrystalline and Nanofilled Polymers." Boulder, CO, July 30 to August 2.

A Special Symposium was arranged at the 34th Annual Conference of the North American Thermal Analysis Society, NATAS held in Bowling Green, KY in honor of my 75th birthday, coupled with an 'Award for Lifetime Accomplishments in Thermal Analysis and Calorimetry' (For more details, see Chapter 10, page 10-8 and Figure 5a).

2006 cont. The meeting started with the participation in the Panel Discussion of the Short Course on "Problem Solving in Thermal Analysis" on Saturday, August 5, 2006, 4:15PM–6:00 p.m. This was followed the teaching of a Section of the Short Course on (A) Application of DSC to the Analysis of Polymers on Sunday, August 6.

During the subsequent meeting, three invited lectures were given in the 'Special Session in Honor of Dr. Bernhard Wunderlich' (B) Thermal Analysis of Macromolecules, A Personal Review: "The Development of the Idea of Thermodynamic Decoupling in Macromolecules." (see Appendix B, Part G) (C) M. Pyda, E. Nowak-Pyda, J. Heeg, H. Huth, C. Schick (Department of Physics, The University of Rostock), A. A. Minakov (Institute of the Russian Academy of Science, Moscow, Russia), and M. L. Di Lorenzo (Instituto di Chimica e Tecnologia dei Polimeri-CNR, Pozznoli NA, Italy. (D) R. Androsch, Effect of Crystallinity and Crystal Perfection on the Rigid Amorphous Structure in Cold-crystallized Poly(ethylene terephthalate). All at the '34th Annual Conference on Thermal Analysis and Applications' of the North American Thermal Analysis Society (NATAS) in Bowling Green KY, August 6–9, 2006.

Trip to Aachen Germany (Including a subsequent vacation travel, with Heidel, including a cruise on the Adriatic See, described on page C-67, below.)

The Glass Transition as Key to Identify Solid Phases, Invited lecture at the DWI at the RWTH Aachen, Germany, October 3, 2006.

2007 Fifty-year Development of the Understanding of Motion and Defects in Macromolecular Crystals Based on Thermal Analysis, Structure Analysis, and Computer Simulation. Invited Lecture at the 234th ACS Meeting in Boston, MA, August 19–23, see page 10-8 and Appendix B. pages B-42–43.

Application of DSC to the Analysis of Polymers. Revised Short Course in connection with the 35th NATAS Conference in East Lansing, MI, Aug. 26–29, 2007, Sunday, August 25, 2007, 8:00–11:15 a.m.

Thermal Properties of Aliphatic Nylons and Their Link to Crystal Structure and Molecular Motion. Lecture contributed to the 35th NATAS Conference in East Lansing, MI, Aug. 26–29, 2007. (See publs. 578a,b in Appendix A)

How to Better Understand Chemistry (And Physics and Materials Science) by Recognizing Only Three Types of Molecules, but Deal with 57 Phases, and Know about the Glass Transitions of Liquids and Crystals. Lecture contributed to the UTK Seminar Series, September 6, 2007.

Differences in Structural and Thermal Properties Between Random and Precisely Structured Copolyolefins Invited lecture at the Meeting on Advances in Polyolefins:, in Santa Rosa, CA, September 23–26, 2007. Lecture cancelled because if illness, but submitted to the proceedings, publ. 579, Appendix A.

2008 Thermodynamics and Kinetics of Crystallization of Flexible Molecules, Contributed lecture to the March Meeting of the APS in New Orleans, LA, March 10–14, Lecture not given due to illness, printed as publ 581, Appendix A.

Travel to the 10th Lähnwitz Seminar in Warnemünde, Germany
(As usual the travel was together with Heidel and coupled with a vacation.)
Thermodynamics and Properties of Nanophases. Plenary Lecture at the 10th Lähnwitz Seminar, on 'Calorimetry in a Nano-scale' in Warnemünde, Germany, June 9–12 (see page 10-4 and publication 584 in Appendix A).

Travel to the ICCT2008 in Warzaw, Poland (not undertaken)
Quantitative Quasi-isothermal TMDSC Techniques To Separate Reversible and Irreversible Thermodynamic Changes in Heat Capacity in the Glass Transition and Melting Range. Invited Lecture at the 20th International Conference on Chemical Thermodynamics, Warszawa, Poland, August 3–8, cancelled due to illness, full lecture printed as publ. 585, Appendix A.

Temperature-modulated Calorimetry of Poly[oxy(benzoate-*co*-naphthoate)]s as Examples of Rotationally Hindered Polymers. Invited lecture at the 36th NATAS Conf. on Thermal Analysis and Applications, in Atlanta, GA, Aug. 18–20. Lecture cancelled due to health problems, publ. 583, Appendix A.

2009 (A) Thermodynamic Description of Condensed Phases. (See publs. 586a,b, Appendix A). In addition (B) Maria Laura Di Lorenzo, Maria Cristina Righetti, Thermal Analysis of the Three-phase Structure of Isotactic Poly(1-butene). (See publs. 587 and 589, Appendix A) Two presentations at the 37th NATAS Conference in Lubbock, TX, September 20–23.

C. MAJOR VACATION TRAVEL AFTER 1954

1954–1991 No major vacation-travel, except in conjunction with business, unless one counts the immigration to the US: 300 mi by train from Frankfurt to Bremerhaven, Germany, followed by 3800 mi to New York City, USA, on with the MS Gripsholm (see pages 5-19–22), and completed by 1550 mi with trains to Hastings, NE (pages 6-1–4).

1992, 1994 1. *Cancún, Mexico.* Described in Chapter 9, pages 9-66–67 and Figures 68–71. All travels were direct round-trip flights. See also page C-61 for a third trip to Cancún in 2004 to attend a one-week conference and to give an invited lecture.

1996 2. *Alaska, US*, Flight to Vancouver, Canada, and travel by cruise ship m/v Crown Princess to Anchorage, AK, via the inside passage (docking at Ketchikan, Juneau, Skagway, and Seward). Within Alaska, flight to the north coast and travel by bus back to Fairbanks and by train via Denali National Park to Anchorage for the flight back. More details in Chapter 9, pages 9-69–72 and Figures 75–79.

1997 3. *Belize in Belize*. Direct flight to and from Belize City, Travel by bus and river boat within Belize and a small-plane excursion to Guatemala. Briefly described in Chapter 9, pages 9-67–68 and Figures 72–74.

1998 4. *Norwegian Fjords*. Flight to Bergen and travel by coastal steamer M/S Nordkapp to Kirkenes with many stops, including the North Cape, as described in Chapter 9, pages 9-73–77 and with Figures 80–87. From Kirkenes we flew to Oslo,Norway. Subsequently to Berlin and then drove to the 5th Lähnwitz Seminar for lectures in Kühlungsborn at the Baltic coast described on page C-52, above. The trip was concluded by traveling back from Berlin to Knoxville.

2000 5. *Hawaii Islands, US*. Vacation trip on the SS Independence, docking at the islands of O'ahu, Kaua'i, Māui, and Hawai'i. Air connection to and from Honolulu, HI. A description of the trip is given in Chapter 9, pages 9-77–79 and with Figures 88–91.

2001 6. *Normandy, France.* Flight to Paris, France, and then by bus to Lisieux, Normandy as headquarter for the Northwestern Alumni College and bus excursions to Bayeux, Giverny, Rouen, St. Hippolyre, Saint-Désir-de-Lisieux, Honfleur, La Cambe, Caen, Pointe du Hoc, Vierville, Colleville-sur-Mer, Avranches, Le Mont-St-Michel, Trouville-sur-Mer, Deauville, and back to Paris for the flight home. (See also Chapter 9, page 9-84 and Figures 93 and 94.)

2002 7. *Caribbean, Panama Canal, Costa Rica, and the Mexican Pacific Coast.* A cruise with the MS Norwegian Sky. The trip began after a flight to Miami, FL, and ended in San Diego, CA, to fly home. Intermediate stops were in Ocho Rios (Jamaica), Oranjestad (Aruba), Panama Canal, Puntarenas and bus to San José (Costa Rica), Acapulco (Mexico), Manzanillo (Mexico), Puerto Vallarta (Mexico). (See also Chapter 9, page 9-84 and Figure 95.)

2003 8. *By ship around Cape Horn.* A cruise with the MS Norwegian Dream, After a flight to Santiago, Chile with sightseeing to the port Valparaiso by bus. Docking points: Puerto Mont (with a tour to Frutillar and Lake Lianquihue), Puerto Chacabuco, then through Canal Darvin and past Chilean Fjords to the Patagonic Chanel and the Straight of Magellan to Punta Arenas (Chile) to visit the penguin reserve Punta Tombo, then via the Beagle Channel with its glaciers to Ushuaia (Argentina). Next, circling the "Cabo de Hornos," and to the British Falkland Islands in the South Atlantic. Then, docking in Puerto Madryn (Argentina) with its wildlife sanctuary Peninsula Valdes, Monetvideo (Uruguay), to reach Buenos Aires (Argentina) and catch a flight back home. (See also Chapter 9, page 9-84, 85 and Figures 96.)

2005 9. *Excursion to Quito (Ecuador) and the Galapágos Islands.* After a flight to and stay in Quito, we flew via Guayaquil to Puerto Baquerizo on San Cristobal Island and boarded the MS Xpedition, a ship of 2,329 GRT, 17 kn cruising speed, and 92 passengers, built in 2001 in Emden, Germany, for a one-week round trip to inspect the unique animal world in the Galapágos Archipelago. From there we went to

Suárez Point on Eapañola Island, to Santa Cruz Island to see the town of Puerto Ayrora, the Darvin Station with its century-old tortoises (lonesome George), Dragon Hill, and Bachas Beach. Next was Bartolome Island (with penguins!), Isabela Island (with the Darwin Lake), Fernandina Island, Rabid Island, North Seymor Island, and back to Santa Cruz Island for the trip back. We crossed the equator four times.

2006 10, *From Aachen to Pula.* This was a one-month trip to lecture (A) in Aachen (see page C-64, above), (B) added travel through Germany (Bergheim, Paffendorf, Iphofen, (C) had our usual vacation in Kössen, Austria (see page 8-50) and (D) followed this with a week's cruise of the Northwestern Alumni along the Adriatic Coast of Italy and Croatia on the MY Monet, starting with a day of sightseeing in glorious Venice (MY = motor yacht, refurbished 1998, 62 passenger, 1,480 GRT). After overnight travel we arrived for an excursion in Ravenna, Italy, then cruised across the Adriatic Sea to Split, Croatia, and followed the Croatian coast with stops at Dubrovnik, Korčula, and Pula, to return to Venice. Being a University Alumni group, we learned a lot about the culture and history of the country, not only about its beauty. From Venice, we managed a direct flight to the US. Finally, the memories ended up in an exquisite 400-file slide show and picture album.

2007 11. *A trip around the world in a private jet in 23 days.* By now, we could find enough time and resources to undertake a true 'trip of a lifetime,' offered to the Northwestern Alumni, referred to on page 9-79. The trip was offered to 90 travelers on a chartered Boeing 757 jet, refitted for the special travel (3,600 mi range, 3 pilots, 2 engineers, one liaison officer, 2 chefs, 9 cabin crew, a physician, and a team of expert lecturers and guides). All inconveniences that normally happen during such travel were anticipated and taken care of. All flights were during daylight hours, all hotels and meals were first class, the standardized (provided) luggage was handled from start to finish, and all of the immigration and customs formality was taken care of (except for occasional signatures). The trip started in (A) Orlando, FL, Feb 24–25, and went through the following stations: (B) Lima, Peru, Feb 25–26; (C) Cuzco, Peru, Feb 26–28; (D) Machu Picchu, Peru, Feb 27; (E) Easter Island, Chile, Feb 28–March 2; (F) Apia, Samoa, March 2–3; (G) Port Douglas, Australia, March 4–6; (H) Port Moresby, Papua New Guinea (PNG), March 6–7, (I) Highlands, PNG, March 7–9; (J) Siem Reap, Cambodia, March 9–11; (K) Agra, India, March 11–12; (L) Dubai, United Arab Emirates, March 12–14; (M) Serengeti, Tanzania, March 14–16; (N) Marrakech, Morocco, March 16–17; (O) Casablanca, Morocco, March 17–18; (P) Orlando, FL, March 18–19. As one can imagine the slides at the end numbered 1,090 of which the 130 best were of exceptional quality. One of Heidel's albums was not enough to holds all the pictures and other mementos, two were needed. A summary is given in Chapter 10, pages 10-13–23 and Figures 16–40.

2008 12. *Sevilla, and Barcelona, Spain.* Again, travel with Northwestern Alumni for a week's stay in Seville, followed by three days in Barcelona, the city connected to Atlanta by direct flights. Besides the beauty and glorious past of Seville, excursions led to Granada, Carmona, Cordoba, and Jeres, all famous Andalusian cities. The whole trip was captured in 500 pictures, illustrating the Roman, Jewish, Moorish, and Christian past, and the present. The best of each seems to be preserved in Andalusia.

2009 13. *A cruise of eleven days from the Atlantic, through the Caribbean Sea, to the Pacific.* Again with Northwestern Alumni by cruise ship. The MS Crystal Symphony (built in 1995, 51,000 GRT, ≈1,000 passengers). The travel went from Miami, FL, to the Atlantic with stops at Sint Maarten, Netherlands, the Antilles Tortola of the British Virgin Islands, and Saint Barthélemy in the French West Indies, to the Caribbian Sea with a stop at Oranjestad on Aruba, Kingdom of the Netherlands, to reach the Panama Canal and cruise the Pacific Ocean to complete the trip in Caldera, Costa Rica. A bus trip brought us to San José, the capital of Costa Rica and the gateway to the plane trip home via Atlanta.