From Biological Macromolecules to Drape of Clothing: 50 Years of Computing for Textiles

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Abstract

The development of computing of structural mechanics of fibres and textiles is linked to the advances in computer hardware and software. The examples cover wool and other fibres, continuous filament and other yarns, micromechanics of woven and other fabrics, and drape of fabrics. The tasks for the 21st century is to develop easy-to-use programs, which will generate a creative interchange between academis and industry, and to use the increased computing power to formulate individual fibre models.

1 Introduction

1.1 Historical

With a few years overlap at each end, the second half of the 20th Century has seen the rise of computing, as indicated below, and the study of the structural mechanics of fibres and fibre assemblies – as well as coinciding with the professional career of the author. An account of the history is instructive, but more attention will be paid to matters of current concern, particularly the *TechniTex* core research in the University of Manchester on the modelling of woven fabrics and the work with Canesis Network Ltd (formerly Wool Research Organisation of New Zealand) on wool and hair. The paper will progress from the nano-scale of molecular structures, through

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the micromechanics of fibres, yarns and fabrics, to the macromechanics of overall performance of products. Almost all the references are to research in association with my colleagues and students. The level of computation in each study is indicated by comparison with the dates in the following list, for which some poetic licence has been taken in order to present a simple story.

- 1950: First programmable computer built by Williams and Kilburn in Manchester, using glass vacuum tubes and post-office relays. Major users only – programmed by changing switches.
- 1960: Batch processing by punched cards. Answers in hours to days. First languages: Mercury and Atlas auto-code in Manchester, Fortran by IBM, etc.
- 1970: Batch processing by teletype input.
- 1980: On-line from terminals to main-frame computer.
- 1990: Personal computers. Advanced languages. Powerful graphics.
- 2000: Global interaction by Internet and e-mail.

In reality, each development ranged over several years, with people and places being at different stages. For example, in July 1967, we made an on-line trans-Atlantic connection through the commercial telex network from Manchester to the textile information retrieval system on a computer at MIT, but it was many years later and with new technology before this became commonplace. Around this time, the Professor of Computing at UMIST saw no place for anything but batch processing on large main-frame computers, but the Professor of Control Engineering was pioneering on-line access to a PDP 10 mini-computer. Milos Konopasek (Hearle et al. 1972) used the PDP 10 for innovative computing techniques for textiles, but it is only now that there is a prospect of industrial usage.

1.2 Routes to Follow

In the beginning, we used computers as little more than powerful calculators to carry out the sums at the end of an investigation. Later it became common practice to carry out complex mathematical analyses and use computing routines for numerical evaluation at the end of the study. Alternatively attempts were made to apply techniques, such as finite element methods, that had been developed in other contexts. Because of the nonlinearity and complexity of textile systems, these academic routes seem doomed to failure as quantitative design tools. For software that will have industrial application, one should start by considering how computing can best deal with the fundamental relations governing a fibre system and how, in a way that is easy to use, it can give useful answers. Getting the right software into industrial use is a necessity, in order to bring about the creative interchange between researchers and users, which has so far been lacking.

Prejudice has to be overcome. The textile industry has an amazing history of empirical development, but the triumph of the practical advances breeds a reluctance to embrace computer-aided design. There are two areas where there were great changes in the last quarter of the 20th Century. One was in computer control of machines, typified by electronic Jacquards and complete production of 3D garments by flat-bed knitting. The other is more relevant to this paper and can be illustrated by a Manchester story. In 1975, textile designers did not like the idea of using computers for the aesthetic design of fabrics by colour and pattern. An earlier grant application by UMIST and the Royal College of Art had failed because it was said that "why do designers need computers, they have pantographs?". Peter Grigg was appointed a Lecturer in Textile Engineering. He obtained second-hand Elliot 903 computers, which were no longer needed by the Navy, and developed a textile CAD system. They were the size of upright pianos and thousands of times less powerful than a modern PC. In the 1980's, TCS Ltd was formed to exploit the system; in the 1990's, the company was bought by Ned Graphics, who now have large stands at textile machinery exhibitions. In this aspect of textile design, the use of CAD has become universal. The same is not true of the engineering design of fabrics. For technical textiles, qualitative trial-and-error, backed by experience, is the norm. One challenge for the 21st Century is to exploit the academic work of the last 50 years and bring in CAD; another is to advance the methodology, stimulated by a creative interchange between industry and academia.

1.3 Approaches to Mechanics

There is one more general point to make. The first approach to modelling textile mechanics has usually been to apply equilibrium of forces and moments. However, almost always, energy methods have proved more powerful. There are various reasons for this, but the most basic is that forces and moments are vector quantities, so that equations are needed for six components. Energy is a scalar quantity, so that there is one basic relation to satisfy. A practical advantage is that it is easier to make useful simplifying assumptions with energy methods. If there is a geometrical relation between macro- and micro-strains, e.g. affine deformation, conservation of energy can be used; if the deformation is undefined, as in buckling, minimum energy or the principle of virtual work is used. Another practical point is that it is usually better to work with mass units (specific stresses in Newton/tex, where tex = g/km, and energies in J/g) than in conventional stress units (Pascals).

2. Molecules to Fibres

2.1 Wool and Hair

Wool and hair have the most complex of fibre structures, Fig. 1, with 10 levels from atoms through a collection of proteins to the form of the whole fibre, as shown in Fig. 2. The explanation of the unusual tensile properties of wool is summarized in Fig. 3 (Chapman 1969, Hearle 2000). The stress-strain curve has Hookean, yield and post-yield regions and, surprisingly, full recovery from large strains, but along a different curve. The structure is a composite of a rubbery matrix around intermediate filaments, which are helically crystalline and characterized by critical and equilibrium stresses for a phase transition to extended chains with 80% extension. This model is so simple as not to need computation. Fortran programs covered more detail of filament/matrix interactions (Hearle et al. 1971). Later, a BBC Acorn microcomputer was used to add time dependence to the model (Hearle & Susitoglu 1985). Other properties are explained by structures at a

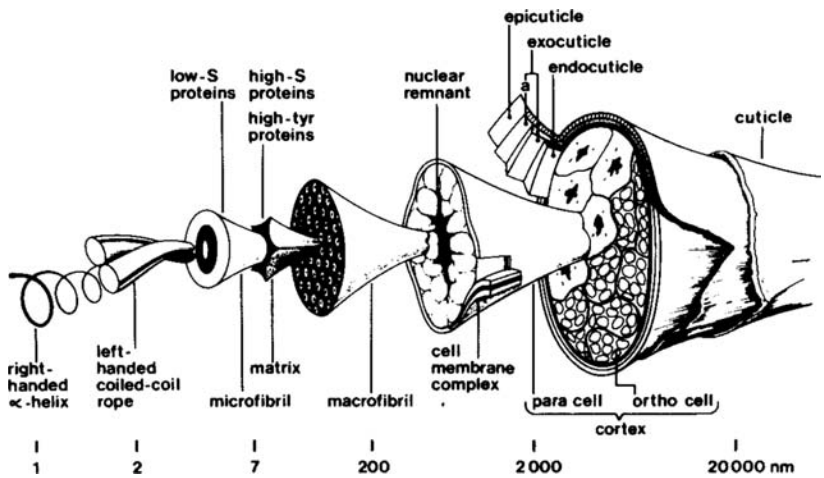


Fig. 1. A view of the structure of a wool fibre, as drawn by Robert Marshall, CSIRO.

coarser level. An important feature is that in the ortho-cortex the macrofibrils are helical assembles of microfibrils, but in the para-cortex the microfibrils are all parallel to the fibre axis. The basic cause of wool buckling into crimped forms had been known since the 1950s, but it was not until it was programmed by a model involving differential contraction of para- and ortho-cortex that there were quantitative graphical predictions (Munro & Carnaby 1999, Munro 2001). A three-component model of stiffness has been modelled (Liu & Bryson, 2002).

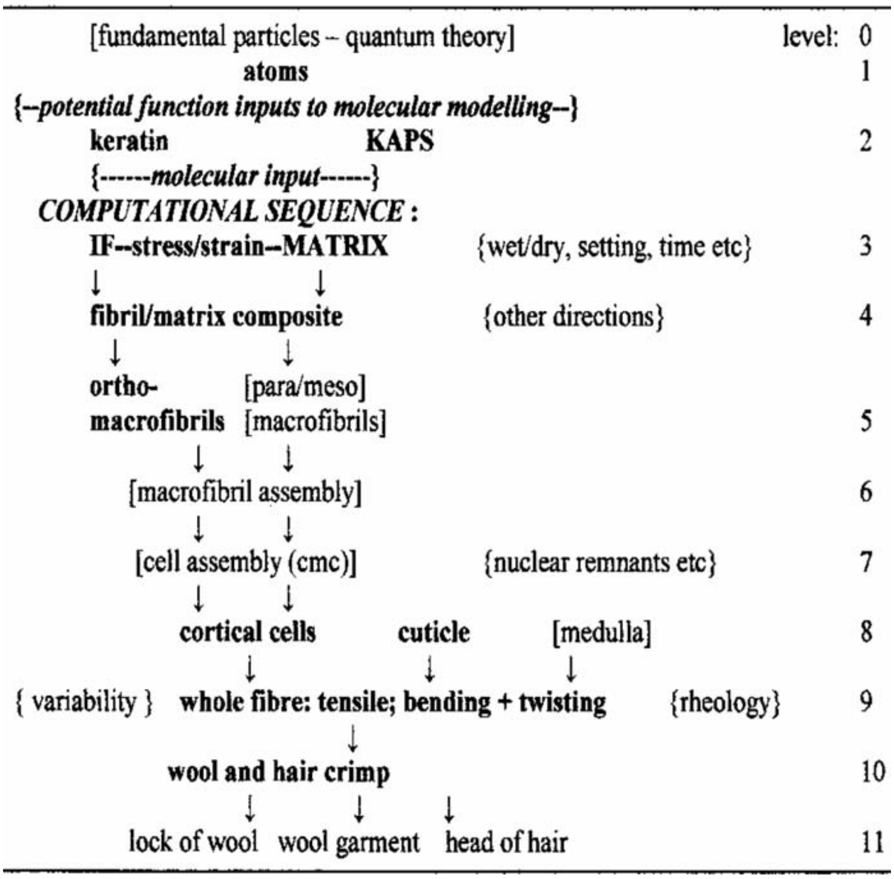


Fig. 2. Levels of structure in wool and hair, with indication of computational scheme for total modelling. Based on (Hearle 2003).

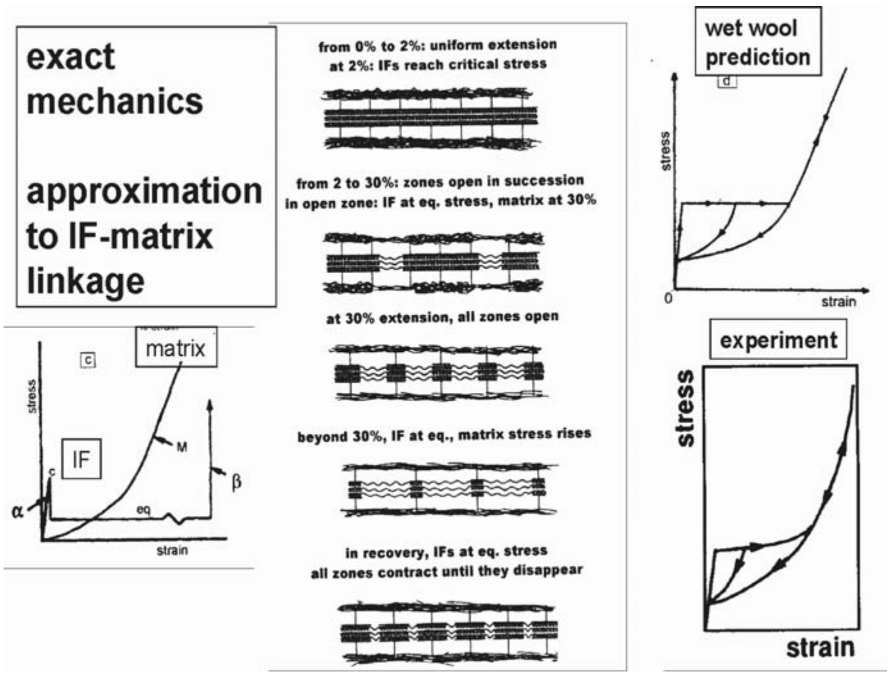


Fig. 3. Mechanics of the wool fibre at level 3 (Chapman 1969, Hearle 2000).

The work to date has been simplified and generic. It gives scientific understanding, but programs should explore the differences between wools, particularly if genetic engineering is used to modify structures. Several computational advances are now needed. A framework program is needed to take outputs from one level as inputs to the next level (Hearle 2003). Some parts of the total model, e.g. a simple dependence on mixture laws, are easy to program. Others are more challenging. At the nano-scale level, computational molecular modelling should be used to determine the full mechanical response of the complex protein assembly in intermediate filaments. Although such modelling has been used to determine protein conformations, the force options, which are in commercial programs, have not been applied to a system of this complexity. The full repeat length is too large to compute, but it should be possible to model separate simpler segments and then link them in a series model. The matrix presents a greater problem, because, although it is critical in determining mechanical properties, its structure is less well known. The development of computational modelling would stimulate an interchange with molecular biologists and applications over a wide field. For the ortho-cortex, the methodology of twisted yarn mechanics needs to be extended to a system in which the matrix contracts on drying, with a consequent shortening of the macrofibrils. At the fibre level, the different properties of para-cortex, ortho-cortex and cuticle (sometimes also meso-cortex and medulla) need to be combined to predict bending, twisting and crimping modes. Another challenge is to model the formation of the structure.

2.2 Other Fibres

Computational modelling is a necessary tool to explain fibre properties. For cotton and other plant fibres with structures determined by nature, a sequence through structural features, summarised in Fig. 4, has been modelled (Hearle & Sparrow 1979). Once again this is a simplified generic treatment and more explicit modelling is needed to predict properties of different cottons. For manufactured fibres, the fine structure has a major role in determining properties, but it has never been engineered deterministically, in the way that both molecules and macroscopic structures are engineered. In the production of melt-spun fibres, fluid and heat flows are computed, but changes in structure result from "twiddling the knobs". Figure 4 includes a view of the possible structure of a nylon fibre. This has been modelled by a network analysis based on energy minimisation. This has been briefly described (Hearle 1991) but not published in detail. The model includes two useful features: the fine structure was treated as a collection of chains emerging from a crystallite; the energy was due to two effects, extension of tie-molecules and change of volume. There is a need and an opportunity for advances in computational modelling of fibre formation, structural forms and prediction of properties.

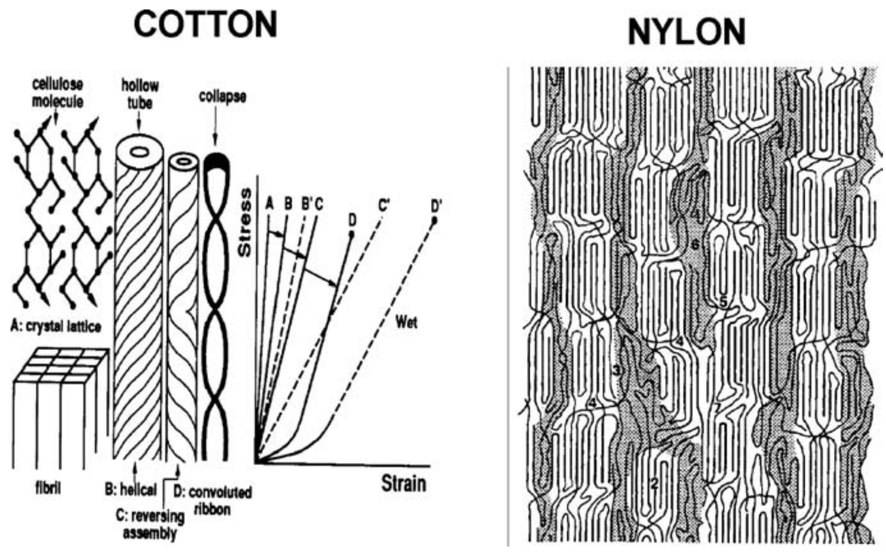


Fig. 4. Models for cotton and nylon. The cotton model is from Hearle (1991); the view of nylon is from (Murthy et al. 1990).

3 Yarns

3.1 Twisted Continuous Filament Assemblies

Twisted continuous filament yarns have a well-defined geometry. Affine deformation relates yarn strain to fibre strain through helix angles. In the 1960's, the force-equilibrium analyses, which were limited to small strains and linear elasticity, were overtaken by large-strain, nonlinear energy methods introduced by Treloar and Riding. This gave a few easily programmed equations (Hearle 1969). Torsion and plied yarns were later included (Hearle & Konopasek 1976).

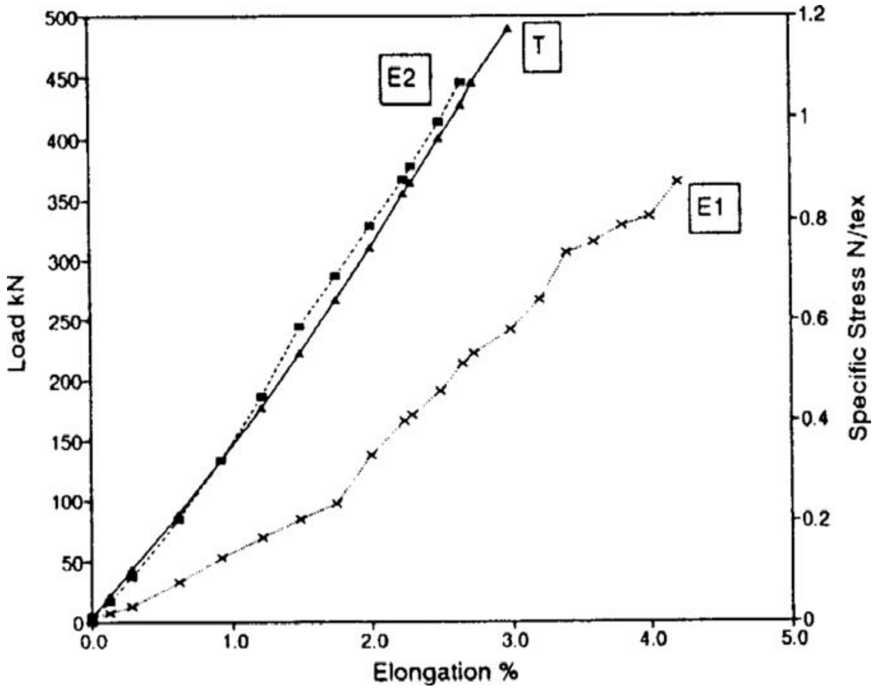


Fig. 5. Use of fibre rope modeller. T was the predicted response for a seven-strand aramid rope. Testing gave E1, but, when the rope was examined, it was found that it had not been made to the correct specification. A correctly made rope gave E2.

Application of the methodology to ropes led to a first use in engineering design by a manufacturer. Fibre Rope Modeller (FRM), developed by Tension Technology International Ltd (TTI) takes account of the multi-level structure of ropes. An earlier DOS version for the US Navy has been converted to Windows. The basic yarn stress-strain curve is input through a set of polynomial coefficients. The program runs through the multiple twist levels in ropes. The output includes details of rope structure, load-elongation curves to break and responses in cyclic loading. In order to determine internal forces, which cause fibre fatigue, the principle of virtual work was used. There are modules for creep failure, hysteresis heating, internal abrasion, and axial compression fatigue. An interesting example of the use of FRM, Fig. 5, shows the good agreement between predicted and tested load-elongation curves (Leech et al. 1993). Strength predictions are typically about 10% higher than observed values due to effects of variability.

3.2 Other Yarns

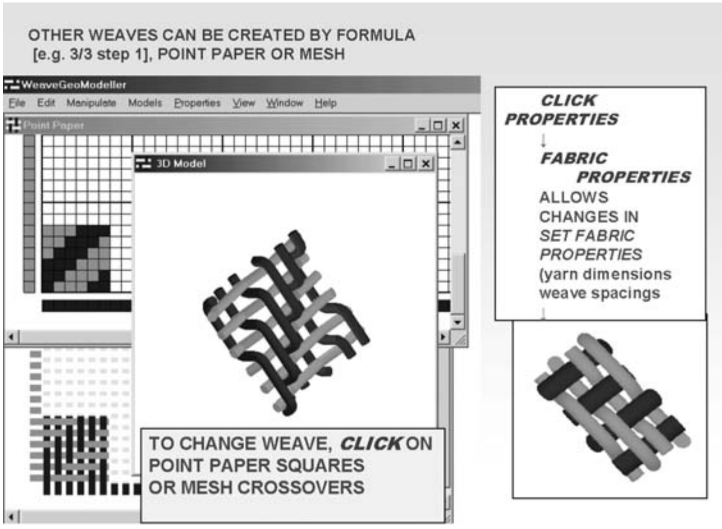
For the simplest staple fibre yarns, the effect of slippage at fibre ends is included (Hearle 1965, Hearle & El-Sheikh 1969). Bulky staple fibre yarns have been much studied from mathematical analysis (Carnaby & Grosberg 1977) to graphical computation (Cassidy 2000), but serious difficulties remain. The underlying problem is that, for quantitative predictions, computational modelling of yarn formation is needed. An open question is whether a global treatment is possible or whether to follow the detail of individual fibre segments.

For false-twist textured yarns, minimum energy computations of the various forms of alternating helices and pig-tail snarls have been carried out (Yegin 1969). For air-jet textured yarns, the entanglements and loops were modelled (Kollu 1985). These academic studies provide a basis for further work, but more is needed for realistic predictions.

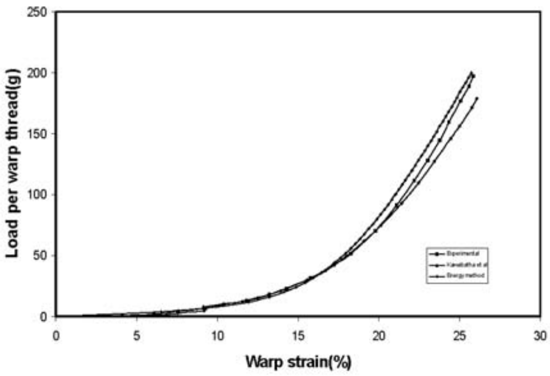
4 Fabric Constitutive Relations

4.1 Woven Fabrics

Almost all the many papers on the mechanics of woven fabrics have used force-and-moment equilibrium, with a saw-tooth model (Kawabata et al. 1973) being the most successful. However, this again seems to be a cul-de-sac, with no outlet to more realistic geometries, large deformations, and nonlinearities. An energy method (Hearle & Shanahan 1978) is the way forward. Through UK DTI-supported technology transfer, this was converted into WINDOWS-based software, *TechText CAD*, in a form for industrial use. Figure 6(a) shows a montage from screens for the input and display of fabric structures, which can be manipulated in various ways. Figure 6(b) shows a comparison of the predicted fabric stress-strain curve with experimental data.



(a)



(b)

Fig. 6. (a) Montage of screens from TechText CAD. (b) Comparison of theoretical predictions with experimental data for cotton fabrics from (Kawabata et al. 1973).

Another program developed by Chen and Porat at UMIST is *Weave Engineer* (TexEng Software Ltd 2005). This covers the basic structure of both hollow and solid 3D weaves, with single layer weaves as a special case, and provides a link to weaving machine settings. These two programs are now being integrated in *TexEng*, which is being developed and marketed by TexEng Software Ltd. Another module provides for easy interchange between the many parameters used to describe fibre, yarn and fabric parameters, including other features such as costings. The intention is to expand *TexEng* to cover a greater range of applications, including knit structures, composites and flow properties.

Computational representation of structural geometry and energy-minimisation for structural mechanics have been advanced in the *TechniTex Faraday Partnership* core research in the University of Manchester to deal with more difficult aspects of woven fabric mechanics (Jiang & Chen 2005, Hearle et al. 2006). The aim is to determine constitutive relations, for a fabric subject to uniform strain. An important feature is the concept of control points. The biaxial deformation of the repeat unit of a fabric is defined by two axial displacements and one transverse displacement, which link an origin to two other primary control points. Additional primary control points are needed to cover the angular change in shear and the curvature in bending and twisting. Secondary control points within the repeat unit are needed to deal with mechanical deformation. Algorithms show up symmetries, which determine the smallest element of a structure to be included in energy minimisation.

Having defined the geometry, the next step is to minimise the sum of extension, bending and flattening yarn energies. Yarn lengths between control points are computed along bent yarn paths. The initial approximation is by B-spline interpolation, which defines curvatures between secondary control points, as illustrated in Fig. 7(a). Twisting would need to be taken into account when yarns follow 3D paths. Yarn flattening has been neglected in the past. Previous studies used symmetrical, circular, race-track or lenticular geometries. Real fabrics show other asymmetrical shapes. A general form is introduced, in which the shape is defined by the radial lengths at a series of angles round the yarn circumference, Fig. 7(b).

Unless the fabric has been totally relaxed, the initial specification of a fabric will not be the minimum energy state under zero applied forces. The first step is thus to minimise the yarn energies to determine this state.

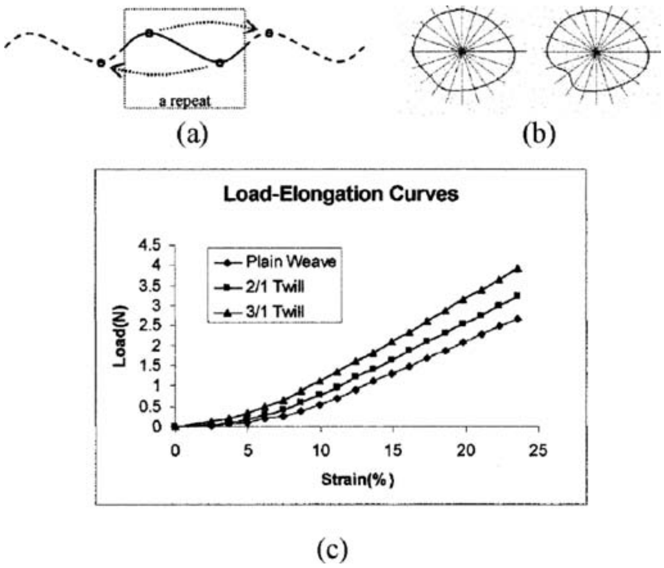


Fig. 7. (a) Curved yarn paths. (b) General specification of yarn shape (Jiang and Chen, 2005). (c) Prediction by Ramgulam of uniaxial load-elongation curve for similar plain, twill 2/1 and twill 3/1 fabrics.

There is a paradox here. The state under zero forces, although attractive as a mathematical origin, is poorly defined. It is easily shifted due to hysteresis or friction. It may be better to define a fabric reference state under small biaxial forces. For the determination of biaxial deformation, the potential energies of applied forces, given by products of force or moment and displacement, must be included. Instead of direct minimisation, it is better to determine the state of internal minimum energy at two closely spaced deformations, and then to equate the energy difference to the work done by the applied force. There are still difficult questions for energy minimisation. Yarn extension energy is known from experiment or yarn modelling. In principle, yarn bending is well understood and bending energy is given by the product of bending moment and curvature. However, the bending stiffness changes from a high to a low value when the fibres start to slip past one another. There will be a different response in free lengths between crossovers and contact regions where there is inter-yarn pressure. Furthermore, in the contact regions, curvature is determined by a combination of bending energy and the less well understood energy associated with change of yarn shape. Flattening energy depends on shear deformations of the cross-section and volume change, and its specification needs new experimental or theoretical methods. Yarn shape may change from contact to free zones. Progress is being made by simplifying in two ways. The first is to carry out energy minimisation with simplified geometries for yarn paths and yarn shapes, so that the minimisation involves fewer terms. Having obtained an approximate solution, the minimisation can be refined by fitting more points along yarn paths and yarn radii. The second is to solve two extreme cases. For monofilaments and hard twisted yarns, we assume that there is negligible change of yarn shape, except through Poisson's ratio due to length change. The curvature in contact zones is then geometrically defined and only the shape in free zones results from the energy szation. Figure 7(c) shows predictions for similar fabrics in three weaves. Very soft yarns deform until the free zone has disappeared, so that it is only necessary to consider the combined bending and flattening energy in contact zones. Further research will lead to ways of treating the following problems: structures between the two extremes; shear and bending deformations; and non-plain weaves, in which side-by-side flattening as well as crossover flattening will occur.

The development of useable computer programs is not a simple matter. Most real needs for structure/property predictions for technical-textile CAD are complicated in yarn and fabric structures and in material responses. Although, in principle, the methodology would cover these complications, in practice, the demands in computer power and time may be too great even for one-off academic demonstrations and certainly for routine industrial use. Clever developments are needed to provide useable programs. The "tricks" should cover:

- efficient programming;
- identification of generally applicable simplifications of geometry and mechanics;
- identification of special cases with particular simplifications;
- recognition of the degree of accuracy required.

4.2 Other Fabrics

Plain knit fabric was modelled using a powerful bending curve program (Konopasek 1970). However, this approach has the same fundamental problem as for woven fabrics, and analogous energy methods need to be developed. Bonded nonwovens were modelled by energy methods based on the orientation and curvature of a representative set of fibre elements (Hearle & Newton 1967; Hearle & Oszanlav 1982), but agreement with experiment was only achieved by the input of measured values of lateral contraction and empirical rules for bond breakage. For needled fabrics, the model added in friction and fibre paths round transverse tufts (Hearle & Purdy 1978). Individual fibre computation will be needed for advances in modelling of nonwovens.

5 Fabric Drape

Early modelling of fabric drape showed its dependence on both bending and shear properties (Cusick 1962). It is the low resistance to shear and area change, that gives weaves and knits their conformability. Computational modelling is needed to achieve a goal of the IT Age, the virtual catwalk. The aim is to enable someone buying an article of clothing on-line to view on a screen how they would really look when moving around in the garment. There are three levels of reality in such simulations. In cartoons, unrealistic distortion is preferred. For realistic animation, in which film-makers have achieved great success, it is only necessary that the image should look right to the viewer. The third level, which is our concern, is to relate the fabric forms to the actual fabric properties and applied forces. This is much more difficult and some IT specialists who came optimistically to the problem have retreated. Leaving on one side the dynamic problem, the first step is to model the quasi-static buckling of textile fabrics in complex situations. Most researchers have attempted to solve the total problem by the use of finite-element or similar methods. However, such programs have not tackled the full anisotropy, which involves three in-plane and three out-of-plane modes of deformation, and the nonlinearity of textile fabrics. The models are limited in their validity, and are horrendously expensive in computer power and time.

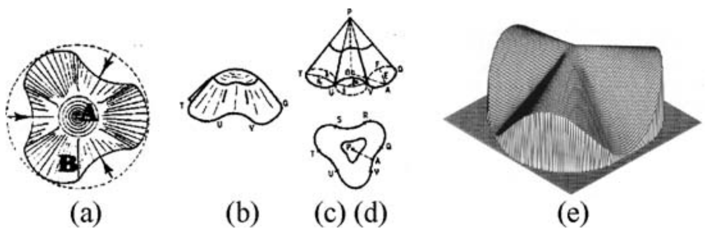


Fig. 8. Threefold buckling. (a) Circle of fabric pushed in from three directions. (b) Upper dome and lower folds. (c) Lower folds modeled as parts of cones. (d) Plan view. (e) Computed prediction of form. From (Amirbayat and Hearle 1986).

A more fundamental approach is needed. Research should elucidate the basics of how fabrics buckle in three dimensions, and find clever ways, which are right for textile fabrics, to build up to the more difficult problems. Threefold buckling of an isotropic, Hookean circular specimen has been modelled by a central dome of double curvature and an outer zone of alternating folds of single curvature as shown in Fig. 8 (Amirbayat & Hearle 1986). The sum of in-plane and out-of-plane strain energies and gravitational energy is minimised, using many simplifications. The approach needs to be improved and extended to remove mathematical infelicities and deal with multiple buckling of real fabrics, but it should show the way forward.

6 Conclusion

At the operational level, the urgent need is for industrial application of the computational techniques developed for fabric structure and mechanics in the last 50 years – to match the advance of CAD for aesthetic design in the last 25 years. It is important that programs should be easy to use and provide the information that is needed in daily operations. Another Manchester development will help this. Many textile problems, notably the way of specifying a woven fabric structure, involve the selection of a small set of independent parameters from a large number of possible parameters that may be used. In order to avoid the need for separate programs for each independent set, *QAS* was programmed to run round a network of equations (Konopasek & Hearle 1972). This later led to the commercial program *TK Solver.* A version of this network facility is included in *TexEng* (TexEng Software Ltd 2005).

At the academic level, the need is for research on treating the more difficult problems in clever ways, which are well adapted to the special features of fibre assemblies. Here the advance in computer power will help. In the 20th Century, we were constrained to treat problems in terms of small repetitive structural units or by statistical distributions of representative elements. In the 21st Century, there is the power to model the behaviour of large numbers of individual fibres or fibre elements. An example is the pioneering study of the compression of a random fibre assembly (Beil & Roberts 2002). Other examples are carpet wear (Hearle et al. 2005) and fabric pilling (Hearle & Wilkins 2006).

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