

Preface

X-ray crystallography is at present the most powerful tool for detailed structural analysis of both single crystalline and micro-crystalline materials. The recent advances in the radiation sources (e.g. micro-focus X-ray tubes), detector technology (CCD, at present also CMOS technology) and most notably in computer programs and CPU power have greatly eased up the routine and non-routine structural analysis, allowing a nearly “black-box” structure solution and refinement. While only a few decades ago a single crystal X-ray diffraction study of a crystalline solid was considered a very tedious and time-consuming task that could be performed only by well-educated and experienced crystallographers, now that is not true anymore. Certainly, in those days X-ray crystallography was not generally accepted as a routine analytical tool for structural analysis, except for well-diffracting small molecule crystals. Meanwhile, the above mentioned advances have had a major impact on the speed and ease of X-ray diffraction analysis. Modern CCD and CMOS area detectors mounted on high-speed diffractometers allow very fast and accurate data collection and processing, so that several, even very large, data sets can be collected and processed in a day. Fast computers also speed up the structure solution and refinement, so that even very complicated solid state structural problems can be tackled within a reasonable time.

This volume does not try to cover the developments of the “classical” crystallography; instead, it intends to put forward those areas which have advanced most during the last two decades, have brought more visibility to these techniques and thus they have broadened the classical views of the crystallography. The volume opens with a comprehensive account on the development of computational crystallography by Professor Angelo Gavezzotti (Milan, Italy) in the contribution “Computational Studies of Crystal Structure and Bonding”. The second chapter “Cryo-Crystallography: Diffraction at Low Temperature and More”, by Dr. Piero Macchi (Bern, Switzerland), introduces the readers to crystallography at low temperatures. Chapter three titled “High Pressure Crystallography” which offers a similar treatise on crystallography under high pressures, where interesting crystallographic events occur, was written by Professor Malcolm McMahon (Edinburgh,

Scotland, UK). Maybe the youngest branch of crystallography, combining photochemistry and X-ray diffraction, *viz.* photocrystallography, is introduced by Professor Panče Naumov (Osaka, Japan) with the chapter “Chemical X-Ray Photo-diffraction: Principles, Examples, and Perspectives”. This concise five chapter volume is closed by an in-depth treatise of the recent advances in the field of X-ray powder diffraction by Professor Kenneth Harris (Cardiff, Wales, UK) titled “Powder Diffraction Crystallography of Molecular Solids”.

On the whole, the contributors to this volume have provided personal accounts on the “new frontier” areas in contemporary crystallography. As editor, I have been truly privileged to have the opportunity to work with my very distinguished colleagues, who have been in the forefront of their research areas for many years. Thanks to their meticulous dedication I am very much convinced that this volume will be a valuable and widening reading experience for researchers and students willing to learn more about the “new frontiers” in crystallography.

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