

Keynote Lectures

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Structural Basis of Cell Regulatory Processes

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High-pressure studies of molecular crystals

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During a long time high-pressure crystallography was dealing more with minerals, metals, and inorganic solids, which were interesting for physics, mineralogy, geochemistry, or materials sciences. Diffraction studies of the organic solids and coordination compounds were limited, although the pioneering work by Bridgeman, Vereschagin, Kabalkina, Fourme, Katrusiak, Allan and some other researchers can be referred to. An enormous progress in the instrumentation and software development for high-pressure research was achieved in the last one-two decades, and this has made diffraction studies possible even for low-symmetry organic crystals. Together with an increased interest in molecular crystals with respect to their applications as materials, devices and pharmaceuticals, this has resulted in a noticeable increase in the number of research groups involved in high-pressure diffraction studies of organic and coordination compounds. This lecture aims to give a general overview of the research in this field, in retrospect and prospect. Attention will be paid, in particular, to the following aspects of research: i) crystallization at high pressure; the crystal structures of high-pressure phases as a tool to study intermolecular interactions; ii) studies of the anisotropic structural strain within the limits of stability of the same phase; understanding the intermolecular interactions; iii) phase transitions at high pressure, thermodynamics and kinetics; iv) pressure-induced chemical reactions; v) effect of pressure on thermal / photochemical reactions.

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Powder diffraction at the nanoscale: structure and defects

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Powder diffraction pattern of nanostructured materials are characterized by broad maxima that overlap widely. This is accentuated if additional defects are present, which destroy the remaining periodicity of the object. Thus the information content that appears to be present is reduced and standard structure determination and refinement procedures do not work any longer. The shape and continuous intensity distribution of these maxima do hold, however, a lot of information on the particle size and defects, which can quantitatively be interpreted by appropriate whole pattern matching.

If the diffraction pattern is measured to very high values of Q , above some 20 \AA^{-1} , a lot of further information about the sample is collected, despite the fact that the diffraction pattern at high Q does not contain any sharp features but broad oscillations at best. With this high Q range, the powder pattern can be transformed via a sine Fourier