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RECENT DEVELOPMENTS IN X-RAY MICROSCOPY

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The properties of X-rays that give them their special role in microscopy are short wavelengths which allows high spatial resolution, high penetrating power and a near absence of impedance mismatch at interfaces which is especially important for imaging of thick hydrated specimens. X-ray energies suited for microscopy provide natural contrast mechanism as well as chemical bond mapping using K-shell and L-shell resonances of many elements in the periodic chart. Therefore, in recent years there have been considerable developments of X-ray microscopes and scanning X-ray microscopes in several countries, using third generation synchrotron radiation sources and zone plate optics as high-resolution X-ray lenses. Besides systems working with X-rays at energies between the carbon and oxygen K edges at 284 eV and 534 eV respectively - the so-called water window - systems have been developed for harder X-rays in the keV-region. X-ray microscopy is currently being used for investigations in biology, medical research, colloid physics, environmental sciences as well as in material research, for example to study domain structures in magnetic materials. For biological applications and especially for X-ray microscopic topographic imaging to reveal 3D-structures cryo X-ray microscopy is of importance.

Keywords: X RAY MICROSCOPY, X RAY MICROSCOPE, X RAY OPTICS

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CRYSTALLOGRAPHY AND ENGINEERING: RESIDUAL STRESS AND MICROSTRUCTURE OF MATERIALS

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Differences between ideal and real crystal structure plays a key role in most applications of crystallography and diffraction techniques to materials science and engineering: grain size, shape and orientation need be considered, together with the presence of lattice defects and residual stresses, resulting from the thermal and mechanical history of the materials. All in all, microstructure and residual stresses are of interest in most materials applications. The present contribution addresses methodological developments in two active and strategic fields: a) Polycrystalline thin films analysis. Texture and residual stress measurements by XRD are necessary to assess thin film properties and stability. Specific methods are required to study the elastic properties, non-uniform texture and residual stress gradients. Research efforts focus on the grain interaction mechanism, which is the key for understanding the elastic and mechanical behavior of thin films and for a correct interpretation of diffraction data. b) Whole Powder Pattern Modeling. Diffraction patterns from polycrystalline materials can be refined without using arbitrary analytical profile functions, on the basis of a detailed physical model of the microstructure, including the contribution of: (i) crystalline grain shape and size distribution; (ii) line defects (in terms of dislocation density, effective outer cut-off radius and screw/edge character); (iii) planar defects, in terms of twin and deformation fault probabilities. WPPM is currently available for cubic (bcc, fcc) and hexagonal (hcp) materials, but an extension to any crystal symmetry is envisaged. Moreover, the WPPM approach can be integrated in a Rietveld program, for a simultaneous structure and microstructure refinement.

Keywords: POWDER DIFFRACTION, RESIDUAL STRESS ANALYSIS, WHOLE POWDER PATTERN MODELLING

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NEW FRONTIERS IN CHARGE DENSITY STUDIES

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Ongoing competitive development of diffraction and computational techniques has resulted in the determination of electron density in the internuclear space of the crystals with a typical uncertainty of 0.03-0.08 $eÅ^{-3}$. Corresponding structural models portray a crystal as a 'sea' of electron density with immersed nuclei. This picture is close to the quantum mechanical description, however, it takes away from canons, which consider a crystal (and molecule) as a set of atoms linked by a network of chemical bonds. Therefore, great efforts were made to establish which atoms, in terms of electron density, are directly bonded and which are not. Additionally, numerous attempts to quantify the atomic and molecular interactions were undertaken. As a result, a language used to interpret the electron density pictures now re-presents the sophisticated and often contradicting mixture of classical and quantum concepts. Certain progress in removing the contradictions has taken place in the last few years. In particular, topological analysis of the electron density was expanded to include the electro-static potential, local energy characteristics and electron localization function. There is a question whether these developments provide new insights on the nature of atomic and molecular interactions. In search of an answer to this question we shall consider the most recent results dealing with electron density features in compounds with different types of chemical bonds. We shall also consider a structural model of electron density in comparison to one, which is geometrical and outline some perspectives of approach such as quantum crystallography and biological applications.

Keywords: CHARGE DENSITY TOPOLOGY

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STRUCTURAL MECHANISMS OF SELF-ASSEMBLY AND POLYMORPHIC SUPERCOILING OF THE BACTERIAL FLAGELLUM

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The bacterial flagellum is made of a rotary motor and a long helical filament by means of which bacteria swim. The flagellar motor at its base rapidly rotates each flagellum to propel the cell movements. The flagellar filament is made of a single protein flagellin, and yet the tubular structure of the filament can form left-handed or right-handed helical forms and switches between these two in response to the twisting force produced by quick reversal of the motor rotation. This allows bacteria to alternate their swimming pattern between running and tumbling, which is essential in their tactic behavior. The flagellum also has a short, highly curved segment that connects the motor and the helical propeller. This segment is called hook. Its bending flexibility allows it to function as a universal joint, whereas the filament is relatively more rigid to work as a propeller. There are two very short segments between the hook and the filament, and these segments are made of protein called HAP1 (Hook Associated Protein 1) and HAP3, respectively. This junction is thought to play a buffering role in connecting the two mechanically distinct structures. We solved crystal structures of core fragments of these proteins. These fragments are missing both terminal regions that are disordered in their monomeric form in solution, but play important roles in stabilizing the polymer forms. All these structures showed interesting implications for the function of each segment, which I will describe in detail.

Keywords: MACROMOLECULAR ASSEMBLY, BACTERIAL FLAGELLUM, MECHANICAL SWITCHING