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Keywords: in-situ powder diffraction, phase transitions, phase diagram

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Structure Solution of Thermal Decomposition Compounds using Laboratory X-rays
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Powder X-ray diffraction at non ambient conditions is developing tremendously, thanks to the rapid progresses in diffraction techniques, methods and software. The present study focuses on the structure solution of inorganic powdered compounds resulting from thermal transformations, using the Bragg-Brentano optics with a conventional X-ray source. Some features related to *in situ* powder data collection are discussed. They include the sample surface displacement, which generates errors on peak positions for pattern indexing, the thermal stability of the products upon heating and the problem of line overlap. Indeed, the latter may arise from diffraction line broadening generated by the crystallite fragmentation during the thermal transformation. This is a major limiting factor for solving the crystal structure, since it strongly affects the structure solution with the direct methods and global optimisation approaches. The influence of the microstructure on the structure solution of the decomposition compound γ-$Zn_2P_2O_7$ is illustrated by a study from simulated patterns.

Representative examples of *ab initio* structure determination of thermal decomposition products will be described, such as those obtained by dehydration reactions of open-framework oxalate and phenylphosphonate materials, and by degradation of nitrate and squarate compounds.
Keywords: structure determination, thermal decomposition, powder diffraction

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Structure Solution of Single-Element Molecules from Pair Distribution Function
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Recent developments of synchrotron x-ray and neutron instruments and acquisition techniques allowed fast and precise measurements of experimental Pair Distribution Functions (PDFs) from molecules, crystals and disordered materials. However, it is usually complicated to extract the structure information from PDF data, and the data processing typically involves a tedious testing of a series of structure models. Therefore it is desirable to find a better way how to analyze PDF data. For single-atom molecules the PDF curves can be converted to a table of inter-atomic distances, which transforms the PDF curve-fitting to a molecular conformation problem. We have developed several algorithms on reconstruction of single atom molecules and tested them with artificial and experimental distance data.
Keywords: ab-initio structure determination, pair distribution function, molecular structure

MS33 SOFT CONDENSED ORGANIC-BIOLOGICAL MATERIALS UNDER PRESSURE

Chairpersons: Roger Fourme, Wilson Poon

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Exploring the Configurational Landscape of Biomolecular Systems under Extreme Conditions
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Lipid bilayers, which provide valuable model systems for biomembranes, display a variety of polymorphic phases, depending on their molecular structure and environmental conditions, such as pH, ionic strength, temperature and pressure. By using spectroscopic and diffraction techniques, the temperature and pressure dependent structure and phase behaviour of simple lipid bilayers as well as binary and ternary (raft) lipid mixtures have been studied. Neutron small-angle scattering, two-photon excited fluorescence microscopy, and FT-IR spectroscopy were used to study also the lateral organization of phase-separated lipid membranes and the influence of peptide incorporation. Moreover, applying the pressure-jump relaxation technique in combination with time-resolved spectroscopic and diffraction techniques, the kinetics of various lipid phase transformations was investigated. The technique was also be applied to study other biomolecular structural transformations, such as protein folding. We present data on the pressure-induced un/refolding of various proteins. A thermodynamic approach is used for determining the stability of proteins as a function of both temperature and pressure and express it as a three-dimensional free energy surface. Morover, the effect of various chaotropic and kosmotropic cosolvents on the temperature- and pressure-dependent structure and stability of proteins is discussed. Finally, recent advances in using pressure for studying misfolding, aggregation and fibril formation (amyloidogenesis) of proteins (e.g., insulin, PrP) will be discussed.
Keywords: high pressure, membranes, proteins

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Probing two Heads Configuration of Heavy Meromyosin by High-pressure SAXS Technique
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We are studying multiple conformations of myosin, by employing the high-pressure X-ray scattering (HP-SAXS). High hydrostatic pressures would shift the equilibrium between conformations. The heavy meromyosin (HMM), a chymotryptic product of myosin, is known to have two heads with one long tail, and HP-SAXS is highly sensitive to the two head orientations. We have carefully optimized the solvent condition for minimal deterioration of HMM both due to aging and radiation damage. The experiments were done at BL45XU-SAXS (SPring-8, Harima) using a compact high-pressure cell [1].

Under 0.1-200 MPa, no structural change was observed that points to that the asymmetric configuration of two heads was rather stable [2]. Above 250 MPa, HP-SAXS pattern of HMM irreversibly changed. At room temperature the change is kinetically controlled, while at -12 °C under 200 MPa HMM structure was equilibrated. The pressure treated samples were all reversible in terms of actin binding and intrinsic Trp fluorescence. We will report on the solution structure of HMM based on HP-SAXS under the low temperature and high- pressure condition.

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Keywords: high-pressure research, SAXS and SANS synchrotron, proteins muscle

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SAXS Investigations of Conformation and Stability of Eye Lens Proteins under Pressure
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We have combined small angle X-ray scattering (SAXS) and a high-pressure cell to study the effect of pressure, temperature and pH,