

of temperature and pressure are presented. As we shall discuss, the experimental findings allow us to relate the intermolecular hydrogen bonding response to the dynamical behavior of the molecular fragments, which justify the ability of the structure to mechanical relaxation.

Keywords: high-pressure phase transformations, amino acids, neutron elastic inelastic scattering

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Structure of ferroic phases in mixed perovskites: Role of multitechnique approach

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The focus of this talk is on the role of multiple-techniques like X-ray powder diffraction, neutron powder diffraction, electron diffraction and Raman scattering in elucidating the structure of various ferroic phases in $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ (PZT), $(1-x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3-x\text{PbTiO}_3$ (PMN-xPT) and $(\text{Sr}_{1-x}\text{Ca}_x)\text{TiO}_3$ (SCT). In synchrotron powder diffraction studies on PZT with $x = 0.520$, one observes a tetragonal (space group $P4mm$) to monoclinic (space group Cm) phase transition only. We have shown that this monoclinic phase transforms further to a superlattice phase in the Cc space group using electron diffraction and neutron powder diffraction data. The Cm to Cc transition is an antiferrodistortive transition involving antiphase rotation of oxygen octahedra leading to small changes in the position of oxygen atoms only, as a result of which the characteristic superlattice reflections are not observable in the powder XRD data but are clearly discernible in electron and neutron diffraction data [1]. The second example in this talk is the structure determination of PMN-xPT for $x = 0.29$. This structure was earlier believed to be rhombohedral on the basis of x-ray powder diffraction data. However, using very high angle reflections in high resolution neutron diffraction data, we have shown that the correct structure is monoclinic in the Cm (MB type) space group [2]. The third example is from SCT system in which the x-ray and neutron powder diffraction data suggest $I4/mcm$ space group for $0.06 \leq x \leq 0.40$ but Raman scattering studies do not support this space group [3].

References:

- [1] D. Pandey, A. K. Singh and S. Baik *Acta Cryst.* A **64**, 192 (2008)
 [2] A. K. Singh D. Pandey and O. Zaharko, *Phys. Rev. B* **74**, 024101 (2006)
 [3] S.K. Mishra et al, *J. Solid State Chem.* **178**, 2846 (2005).

Keywords: PZT, PMN-xPT, ferroics

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Probing the structure of heterogeneous diluted materials by diffraction tomography

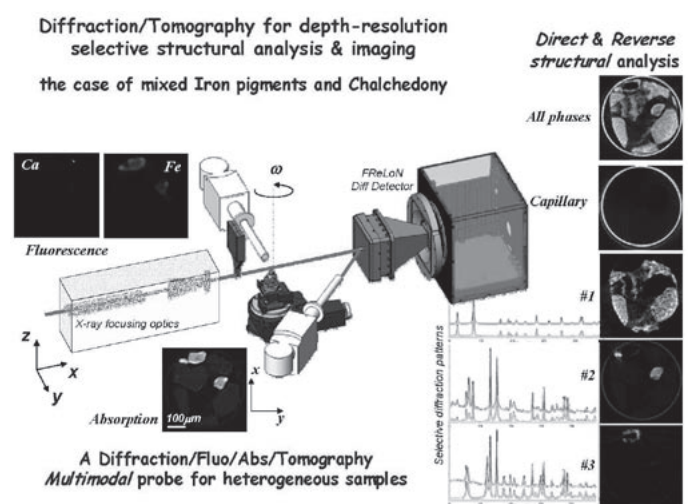
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We evidence the potential of coupling pencil beam tomography with X-ray diffraction to examine unidentified phases in heterogeneous materials and to overpass the relatively low detection limit of X-ray diffraction. The demonstration is performed on a heterogeneous powder containing chalcedony and iron pigments (see figure). Furthermore we will also present the 3D phase selective reconstruction of a high-pressure pellet containing several carbon phases. The present method allows a non-invasive structural refinement with a weight sensitivity of one part per thousand. It allows the extraction of the scattering patterns of the amorphous and crystalline compounds with similar atomic densities and compositions. Furthermore, such a diffraction-tomography experiment can be carried out simultaneously with X-ray fluorescence, Compton, and absorption tomographies, allowing a multi-modal analysis of prime importance in materials science, chemistry, geology, environmental science, medical science, paleontology and cultural heritage [1].

[1] P. Bleuet, E. Welcomme, E. Dooryh e, J. Susini, J-L. Hodeau, P. Walter, *NatureMaterials* (2008) in press , URL: <http://dx.doi.org/> , DOI: 10.1038/nmat2168



Keywords: diffraction methods, tomography, diffraction imaging of heterogeneous specimens

MS.27.3

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Electronic behaviour of materials from combined X-Ray, neutron diffraction and Compton scattering

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High resolution X-Ray (gamma Ray and more recently convergent electron beam) diffraction has been widely used to get electronic charge density behaviour in solids, including complex inorganic systems and up to biological molecules. This research is challenging towards theoretical modelling of condensed matter. Recent time resolved studies open a new area, through the out of equilibrium time dependent charge density . Magnetic neutron scattering allows for accessing magnetisation and mainly spin density . The applications towards molecular and nano magnetism are very timely . Electronic behaviour can also be approached in momentum space,

through Compton scattering, leading to highly complementary information, the momentum density. Those three functions convey distinct information, and are connected through the one particle reduced density matrix (1RDM), the key information for describing any microscopic property of a system, at least within a mean field approach. We are developing a joint analysis of those different experiments when available. It involves defining model parameterisation of the 1RDM. The method of joint refinement from independent and complementary experiments will be discussed, with applications to inorganic and molecular materials. One main interest of such approach consists in modelling condensed matter as a superposition of fragments with a flexible transferability among similar compounds. Various examples will be given, concerning inorganic complex compounds and also systems with pharmaceutical applications.

Coordinator of CEDA research ANR project, together with D. Luneau, (LMI, Lyon), B. Gillon (LLB, CEA), M. Souhassou (LCM3B, Nancy), Y. Sakurai (Spring8, Japan)

Keywords: electron density, modeling properties, fragment transferability

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Complex texture and structure of shocked quartz mineral with graphite grains

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Quartz mineral formed by shock impact reaction from dynamic high pressure and temperature (about several thousand degree) is still unknown so far. This paper presents detailed data with electron microscopy and X-ray structure analyses of shocked sample (SQ12 from impact crater), which are compared with normal single crystal of rock-crystal (RQ in Japan) as follows: 1) Field-emission scanning electron microscopy (FE-SEM) with analytical device indicates that shocked quartz with shocked lamellar texture (SQ12 sample) is assemblages of irregular micro-grains of 100 nm to 3 micrometers, where carbon grains with 300 nm to 10 micrometers are involved along shocked lamellar planes, and grain-boundaries of micro-domains of quartz. 2) The EDX spectra of FE-SEM indicate that carbon grains contain some silica contents as impurities from silica-rich target rock at impact event. The present data suggest that X-ray diffraction (XRD) of powdered sample SQ12 shown as weak and diffuse X-ray intensity peaks is considered to be also effect of overlapping XRD peaks of graphite carbon. 3) X-ray structure analyses of these impact sample SQ12 compared with quartz RQ, indicates effects of irregular assemblages and shocked lamellar planes of quartz silica and graphite carbon. Structural data of shocked quartz silica formed relatively quenching process (from high-temperature and pressure) show similar data of twinning crystal data of mineral formed relatively slow-cooling process of melting. 4) Dynamic impact reaction from high pressure and temperature makes characteristic crystal data of quartz with various textures of domains, lamellae and coexisted foreign minerals as dynamic quick-cooling process.

Keywords: shocked quartz mineral, irregular grains, graphite carbon mixing

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The effect of structural and compositional details on physical properties of new double-perovskites

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Double perovskites of general formula $A_2MM'O_6$ are a class of compounds, crystallizing in a superstructure of the perovskite type with an ordered distribution of M and M' cations on crystallographically distinct sites. The physical properties of these compounds depend strongly on details of the chemical composition and subtle structural features: Depending on the ionic radii of the M and M' ions a significant degree of cation disorder will be observed on these sites, quantified by the relative amount of M-ions on the M'-site and vice versa. A cation disorder of 0% refers to a perfectly ordered structure, while a cation disorder of 50% means a completely random distribution of the M and M' ions, representing a normal perovskite $A(M,M')O_3$. In addition to this cation disorder, oxygen vacancies can be of high relevance for the physical properties, especially if one of the elements can exist in different formal oxidation states. A very often applied approach to vary the physical properties is to substitute the A-site with another element A' with a different oxidation state and hereby changing the valencies on the M and M' sites. The interpretation of the resulting properties requires a sophisticated characterisation of the obtained material, which can only be provided by a multitechnique approach. We will report on some new examples of double perovskite compounds with $A=(La^{3+}, Sr^{2+})$, M a 3d transition metal and $M' = Ir, Ru$ or Re . The underlying crystal structures will be determined by several complementary methods (e.g. diffraction using synchrotron and neutron radiation, XPS, ICP-OES, oxygen determination) to resolve any ambiguity within the above mentioned structural degrees of freedom and correlate composition and structure with the resulting magnetic properties.

Keywords: perovskites, diffraction using synchrotron & neutron radiation, site disorder

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Induced structural diversity in magnetic molecular materials

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Although the basic aim of crystallography is to determine the crystal and molecular structure of crystalline solids, much more important and interesting is the relationship between structural features and physical properties. Understanding what makes a material perform its 'function' is essential for the design of new materials with novel or enhanced properties. Within this context, new opportunities for the development of novel electronic devices may arise from the