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

MS.27.1

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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 $Pb(Zr_xTi_{(1-x)})O_3$ (PZT), $(1-x)Pb(Mg_{1/3}Nb_{2/3x})O_3$-$xPbTiO_3$ (PMN-xPT) and $(Sr_{(1-x)}Ca_x)TiO_3$ (SCT). In synchrotron powder diffraction studies on PZT with x = 0.520, one observes a tetragonal (space group *P*4*mm*) to monoclinic (space group *C*m) 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 *I*4/*mcm* space group for $0.06 \le x \le 0.40$ 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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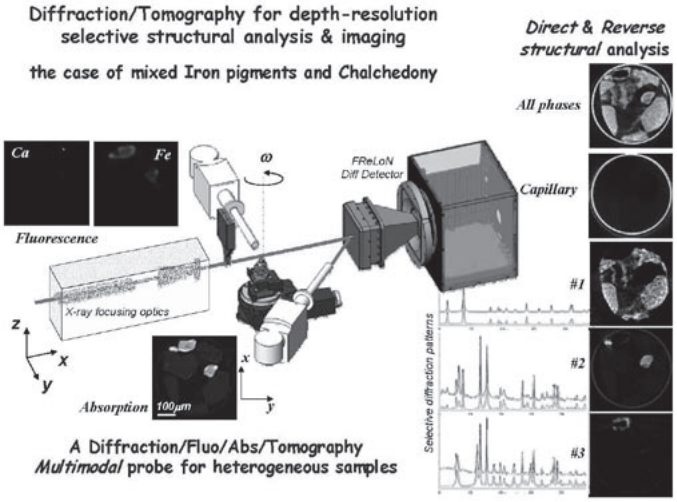
We evidence the potential of coupling pencil beam tomography with X-ray diffraction to examine unidentified phases in heterogeneous materials and to overpass the relatively low detection limit of X-ray diffraction. The demonstration is performed on a heterogeneous powder containing chalcedony and iron 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. Dooryhée, 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

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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,