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Local polarizations and the interaction between them play a crucial role in the relaxor behavior of relaxor ferroelectric $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN). We report the temperature evolution of the local and medium-range crystal structure of PMN from 1000K to 15K using neutron pair distribution function analysis [1]. We present evidence for both local atomic displacements (local polarization) and for medium-range (~ 5 Å - 50 Å) ordering, called polar nanoregions (PNRs). These medium-range correlations are modeled using rhombohedral symmetry, enabling for the first time an estimate of the temperature dependence of the volume fraction of the PNRs. We show that this fraction steadily increases from 0% to a maximum of ~30% as the temperature decreases from 650K to 15K. Below T ~ 200K the volume fraction of the PNRs becomes significant, and PNRs freeze into the spin-glass-like state.

[1] Jeong I.-K., Darling T. W., Lee J. K., Proffen Th., Heffner R. H., Park J. S., Hong K. S., Dmowski W., Egami T.. *Phys. Rev. Lett.*, *in press*.

Keywords: relaxor, medium-range ordering, PDF

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Getting the most from Total Scattering

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Total scattering, an extension of the powder diffraction method, is increasingly being used to study crystalline materials. The unique combination of Bragg and diffuse scattering can be used to determine both the average structure and the short-range fluctuations from this average within a single experiment. To maximise the structural information from such data three-dimensional atomic models consistent with all aspects of the data are required. Here I present a technique for producing such models based on the reverse Monte Carlo (RMC) method. The existing RMC method has been expanded to take explicit account of the Bragg intensity profile from crystalline materials [1].

Analysis of the RMC-generated atomic models gives much more detailed information than is available directly from the data. I will give several examples where this method has been used to successfully study the structure and dynamical disorder of materials including those with the perovskite structure [2], those showing negative thermal expansion and molecular crystals. I will also show examples of low-energy phonon dispersion curves obtained from the models [3].

[1] Keen D. A., et al, *J. Phys.: Cond. Matt*, 2005, **17**, S15. [2] Hui Q., et al, *J. Phys.: Cond. Matt*, 2005, **17**, S111. [3] Goodwin A. L., et al *Phys. Rev. Lett.* **93**, 075502, 2004.

Keywords: reverse Monte Carlo, structural simulation, neutron X-ray scattering

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Characterisation of Nanoparticles

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Powder diffraction patterns of ZnO as well as CdSe/ZnS core shell nanoparticles were obtained and analysed with respect to particle size, defect density and local structure. The pair distribution function was successfully used to analzse the local structure.

The ZnO pattern was refined by the Rietveld method using a wurtzite structure. The moderate agreement shows that the particles are of anisotropic shape and have a stacking fault density of some 20%. The nanoparticles were modelled and size, shape, stacking fault density, positional and displacement parameters fitted to the powder pattern by means of the Debye formula as well as to the respective experimental Pair Distribution Function. The two methods give similar results of some 3.5 nm parallel [100] and 2.5 nm parallel [001] in size.

The CdSe nanoparticles and CdSe/ZnS core-shell nanoparticles show diffraction patterns that qualitatively fit to a wurtzite structure. The size of 3 nm as well as stacking fault density of 25% and distortions at a surface layer degrade the powder pattern. The pattern of the CdSe/ZnS core-shell nanoparticles are widened at the high 2θ side compared to the pure CdSe nanoparticles. The smaller metal-anion distance (Zn-X=0.235 nm, Cd-X=0.27 nm) causes a distortion of the whole particle.

Keywords: nanoparticle, pair distribution function, local structure

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MS75 SURFACES

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Electromagnetic Wave Tunneling Through a Barrier With Periodical Structure

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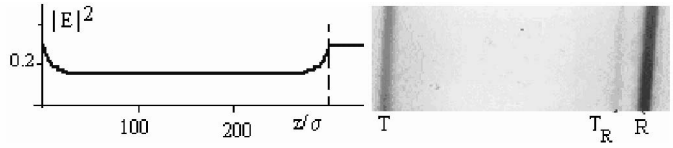
We discuss specific features of electromagnetic wave localization inside specimen with periodical structure in diffraction regime. The problem was solved by Hambartsumian's layer addition method modified for cholesteric liquid crystal layer (CLCL)[1]. Experiment for a perfect single crystal of silicon was fulfilled when x-ray beam was reflected from atomic planes $(2\bar{2}0)$. We reveal an interesting manifestation of electromagnetic wave tunneling through barrier with periodical structure, namely, we theoretically and experimentally showed that when electromagnetic wave propagated through the barrier in the Bragg regime the wave field in the specimen was localized near the specimen boundaries, while it was practically absent inside the sample. Using this we explained the fact (observed in experiment) that absorption and scattering inside the sample are practically absent, and that reflection takes place only from the two surface layers of the sample. Fig. 1 shows electromagnetic wave intensity distribution in CLCL in the Bragg diffraction regime (a) and x-ray sectional photograph from the two block silicon systems, when the primary beam (which is reflected from the first block and incident onto the second block) then forms three beams; R is reflected from the entrance surface, T is the transmitted beam and T_R is reflected from the side surface.



[1] Gevorgyan A.H., et al., *Opt. Spectrosc.*, 2000, **88**, 647.

Keywords: diffraction, tunneling, surface physics

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Holographic Methods for Surface Crystallography

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A hologram stores information about the amplitude and phase of a wave in an interference pattern with a known reference wave. The unknown wave may be recovered through a process known as reconstruction. It has been suggested that many diffraction patterns, e.g. those formed by photoelectrons, or low energy backscattered electrons may be capable of a holographic interpretation, and