Acta Cryst. (2002). A**58** (Supplement), C229

X-RAY DIFFUSE SCATTERING IN THE FERROELECTRIC MATERIALS

A. Pietraszko K Lukaszewicz
Institute for Low Temperature and Structure Research Polish Academy of Sciences, Wroclaw, Poland

Ferroelectricity is directly coupled with the ordering of crystal structure. For discontinuous transitions the X-ray diffuse scattering (XDS) in the low and high temperature phase can be expected quite different. In the continuous transition; the transformation is due to progressive and cooperative disordering. In the ferroelectric structures containing polar groups the increasing temperature produces a disordering of these groups. Above transition point the structure becomes centrosymmetric in the macroscopic scale but still contains small polar nanodomains.

Our recent results obtained by the recording of XDS using the X-ray diffractometer with the CCD detector will be presented. In the quantum paraelectric crystals in the centrosymmetric para-phase the XDS is associated with ferroelectric polar nanoregions. In the relaxor materials with diffuse transformations the polar nanoregions in the para-phase have been found. The XDS study of the structural arrangement and glass-like transition behavior of relaxor $Pb(B'_{0.5}B'_{0.5})O_3$ where B'=Nb; Ta shows the occurrence of the freezing antiferro- and ferro-electric fluctuations and the small nano-regions with ordered B'/B' cations.

Although the sodium nitrate ($NaNO_2$) crystal is typical order-disorder ferroelectrics with the simple structure; the arrangement of atoms in the nano-domains in the para-phase in the para-phase associated with the modulation wave and with the polar nano-region was found. The results of XDS studies of ferroelectric SbSI crystals with the pseudo Jahn-Teller transition and the semiconducting and weak ferroelectric Sb_2S_3 crystals will be presented.

The work was supported by the Polish State Committee for Scientific Research no 2 PO3B 136 17

Keywords: DIFFUSE SCATTERING, FERROELECTRICS, PHASE TRANSITIONS

Acta Cryst. (2002). A**58** (Supplement), C229

MAGNETIC DIFFUSE SCATTERING FROM Zn-Mg-RE and Cd-Mg-RE (RE: RARE-EARTH) ICOSAHEDRAL QUASICRYSTALS

T. J Sato[1,2] H. Takakura[2] A. P. Tsai[2] K. Ohoyama[3] K. Shibata[3] K. H. Andersen[4]
[1]NIST Center for Neutron Research, NIST, GAITHERSBURG MARYLAND USA [2]National Institute for Materials Science, Japan [3]IMR, Tohoku University, Japan [4]ILL, France

Recent discovery of magnetic quasicrystals in the Zn-Mg-RE and Cd-Mg-RE (RE: rare earth) alloys enables us to study behavior of magnetic moments (or spins) in a quasiperiodic lattice. Magnetic susceptibility suggests that these quasicrystals are classified as a spin-glass, i.e., the spins randomly freeze at low temperatures. However, neutron diffraction detects strong magnetic diffuse scattering at low temperatures. This indicates significant development of the short-range magnetic ordering, and thus discriminates the quasicrystals from typical random spin-glasses. In the present study, we try to obtain some insight into local spin configurations in the short-range ordered region; a primary focus is situated on Zn-Mg-RE since the single-quasicrystal neutron diffraction data are available. The data indicate the correlation length of about 2nm, and thus, the short-range ordering is presumably confined in a certain small structural unit of this size. As such a structural unit, we propose a dodecahedron; a calculated ground state of Heisenberg spins on the dodecahedron well reproduces the observed diffuse scattering pattern. Further support is obtained from inelastic scattering study; a strongly-localized inelastic scattering peak observed at 2.5 meV can be explained by the inelastic modes of the dodecahedral spin cluster. These results strongly suggest that the magnetic ordering, as well as the magnetic fluctuation, in the quasicrystals is likely to be confined to a small structural unit with high symmetry, which is, in the present case, the dodecahedron. Quite similar neutron diffraction results, but obtainable only for powder samples, suggest the same scenario for the Cd-Mg-RE quasicrystals.

Keywords: NEUTRON SCATTERING QUASICRYSTAL MAGNETIC SCATTERING

Acta Cryst. (2002). A**58** (Supplement), C229

DIFFUSE SCATTERING BY Fe-Ni SOLID SOLUTION ALLOYS

G..E. Ice[1] C.J. Sparks[1] J.L. Robertson[2] R.I. Barabash[1]
[1]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge TN 37831-611 USA [2]Solid State Division,Oak Ridge National Laboratory, Oak Ridge TN 37831-611

Precision static displacements and chemical correlations were recovered from diffuse x-ray measurements on Fe-Ni solid solution alloys. Local chemically-specific atomic pair correlations are obtained with the 3l method. In computer simulations, atoms were distributed on a FCC lattice to match the experimentally derived Warren-Cowley pair correlation parameters. Attempts to model the essential features observed in the experiments are discussed. The preference for unlike first neighbor pairs causes the diffuse scattering to peak at the super lattice reflections for an ordered structure and the experimental measurements indicate the presence of plate-like domains with diameter of about 3 unit cells and a thickness of 1-2 unit cells aligned in the [100] direction. Local ordering can be a precursor to the lower temperature equilibrium structure, which may be unattainable because of slow atomic diffusion. Static displacements waves related to such domains strongly influence the scattering intensity around fundamental and superstructure positions.

Keywords: DIFFUSE SCATTERING, SHORT RANGE ORDER, PAIR CORRELATIONS

Acta Cryst. (2002). A**58** (Supplement), C229

STRUCTURES, ORIENTATIONAL ORDERING AND PHASE TRANSITIONS IN C_{70} SINGLE CRYSTALS

R. Moret S. Rodts P. Launois
Laboratoire de Physique des Solides, CNRS - University of Paris-Sud, Orsay , France

Solid C_{70} forms several polymorphs and undergoes sequences of temperature-induced phase transitions due to the orientational ordering of the elongated fullerene molecule. We have studied several C_{70} single crystals, grown from the vapor phase, using diffraction and diffuse scattering techniques at room and low temperature. We find that cubic and hexagonal close packed (hcp1 and hcp2) structures coexist at room temperature. The two hexagonal varieties correspond to uniaxial (hcp1) and isotropic (hcp2) orientational disorder of the elongated C_{70} molecules. These distinct disorder types give rise to specific diffraction and diffuse scattering intensity distributions, which are satisfactorily fitted by computer simulations. Precursor diffuse scattering is observed in hcp1, above the transition (at about 290 K) towards the monoclinic low temperature phase, whose structure is re-examined. In hcp2 we observe diffuse scattering features, which we attribute to the coupling between orientational and translational molecular degrees of freedom [1], as predicted by microscopic theories [2]. Quantitative analysis of this diffuse scattering is of prime importance for the understanding of the microscopic interactions in the non-spherical fullerenes. The recent observation of superconductivity in electron-doped C_{70} [3] clearly demonstrates the need for a better knowledge of these fundamental properties.

Reference
[1] P. Launois and R. Moret, J. Phys. IV France 10, Pr3-193 (2000).
[2] R. Sachidanandam and A.B. Harris, Phys. Rev. B49, 2878 (1994) ; A.K. Callebaut and K.H. Michel, Phys. Rev. B52, 15279 (1995).
[3] J.H. Schön et al. Nature 413, 831 (2001). S. Rodts' present address : LMSGC 2, allee Kepler 77420 Champs-sur-Marne, France.

Keywords: C70 ORIENTATIONAL DISORDER PHASE TRANSITIONS