simple case, e.g., spherical particle-particle correlation. The particle-particle correlation effect without the atomic correlation gives us a background in PDF. One of important points in PDF analysis is to include background in a diffraction pattern. Interestingly, the background in PDF gives us information of particle-particle correlation when there is no atomic correlation between the particles. These three effects will be discusses by using PDF data sets of TiO_2 nanoparticle [6], $Ge_2Sb_2Te_5$ nanoparticle embedded in amorphous matrix [8], and C60 powder samples.

References

[1] T. Egami and S. J. L. Billinge, Underneath the Bragg Peaks: Structural Analysis of Complex Materials, Pergamon, Amsterdam, 2003.
[2] M. Gateshki, et al., Z. Kristallogr. 222 (2007) 612.
[3] P. Juhas, et al., Nature 440 (2006) 655.
[4] B. Gilbert, et al., Science 305 (2004) 651.
[5] http://discus.sourceforge.net
[6] K. Kodama, et al., Acta Cryst. A 62 (2006) 444 .
[7] R. C. Howell, et al., Phys. Rev. B 73, (2006) 094107.
[8] S. Shamoto, et al., Jpn. J. Appl. Phys. 45-11 (2006) 8789.

Keywords: PDF analysis, finite size effect, particle-particle correlation

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High pressure studies of planetary ices

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In the context of the outer solar system, the ices (water-ice, ammonia, methane and mixtures of these) are minerals. Their high-pressure behaviour is thus crucial to models of the evolution of planets such as Uranus and Neptune and planetary satellites like Titan, Ganymede and Triton in the same way as the properties of ferromagnesious silicates are basic to models of the Earth. Over the past ten years, access to high-quality x-ray and neutron diffraction data has provided a wealth of new information on high-pressure structures and phase relations for many of the ices. This has greatly enhanced our understanding of these systems and placed models of planets on a firmer basis. In my talk, I will describe some of the results that I and co-workers have obtained in the methane, methane-water, ammonia and ammonia-water systems and describe the consequences for planetary models.

Keywords: high-pressure diffraction, high-pressure neutron diffraction, planetary interiors

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Nucleation and growth of ice XI -Study suggests the existence of ferroelectric ice in the Universe-

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From neutron powder-diffraction experiments, we have studied the growth process of ferroelectric ice XI with deuteron-ordered arrangements. We measured time-resolved neutron diffraction of compressed KOD or NaOD doped D_2O-ice. We observed the growth of ice XI at 58 - 74 K. The mass fraction f (the ratio of mass of ice XI to that of the doped ice) linearly increased with time for about 5 days. The de-transformed ice Ih, obtained after warming above the transition temperature of 76 K, retransformed to ice XI at 60 -66 K. The observed increase of f with time is in good agreement with the nucleation process of the ordering and the constant growth of the ordered domain. The results suggest that large quantities of ice on cold icy bodies (such as Pluto and Charon) in our solar system are able to transform to ice XI, which may be detectable by space telescope and planetary exploration.

Keywords: neutron powder diffraction, time-resolved structural studies, ice structures

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High-pressure phase transitions of deep Earth materials

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Recent developments in synchrotron XRD measurements combined with laser-heated diamond-anvil cell (LHDAC) techniques have enabled us to search for a novel phase transition at extremely high pressure and temperature. A phase transition from $MgSiO_3$ perovskite to post-perovskite was discovered through a drastic change in XRD patterns above 120 GPa and 2500 K, corresponding to the condition in the lowermost mantle (Murakami *et al*., 2004; Oganov and Ono, 2004). A pressure-induced phase transformation from ABO_3-type perovskite to any denser structures was not known at that time. This new $MgSiO_3$ polymorph called post-perovskite has an orthorhombic symmetry (space group: *Cmcm*) with a sheet-stacking structure. The Mg site in post-perovskite is smaller than that in perovskite, which results in a volume reduction by 1.0-1.5% from perovskite structure. The electrical conductivity of post-perovskite is higher by three orders of magnitude than that of perovskite at similar pressure range (Ohta *et al*., 2008). This is likely due to a shorter Fe-Fe distance in post-perovskite structure, while conduction mechanism is yet to be further examined. Phase transition boundary between perovskite and post-perovskite has been determined in a wide temperature range up to 4400 K at 170 GPa (Tateno et al., 2008). Phase relations of Fe alloys have been also studied at core pressures (>135 GPa), although the generation of high temperature is more difficult at higher pressures. A new high-pressure B2 phase of FeS was recently discovered above 180 GPa (Sata *et al*., 2008). The Fe-Ni alloys have a wide pressure-temperature stability field of fcc phase at the core pressure range, depending on the Ni content (Kuwayama *et al*., 2008).

Keywords: high-pressure phase transformation, perovskite oxides, iron compounds