contractions and anomalous domain structures were observed. By substiduting D_2O at fixing the water concentration, the anomalies disappeared gradually. On the other hand, the quenched mixtures of RTILs-H_2O show a curious "*double glass transition*".[6-9] Bonding nature of hydrogen plays an important role both on crystal and glassy states.

Recently, we found hierarchal structure in the [DEME][BF_4]-H_2O system by small angle X-ray scattering, "prepeak" and principal peak on the X-ray diffraction and optical absorption in UV-vis region.[10] Even at liquid state, water-mediated heterogeneous fluctuations are dominant. Furthermorre, nearly-free hydrogen bonded water in Raman spectra is detected below 80 mol% H_2O mixtures. Water network over the medium-range is key to comprehend the complicated behaviors.

[1] Y. Imai, H. Abe, T. Goto, Y. Yoshimura, S. Kushiyama, H. Matsumoto, *J. Phys. Chem. B* **2008**, *112*, 9841-9846. [2] Y. Imai, H. Abe, T. Goto, Y. Yoshimura, Y. Michishita, H. Matsumoto, *Chem. Phys*. **2008**, *352*, 224-230. [3] Y. Imai, H. Abe, Y. Yoshimura, *J. Phys. Chem. B* **2009**, *113*, 2013-2018. [4] H. Abe, Y. Yoshimura, Y. Imai, T. Goto, H. Matsumoto, *J. Mol. Liq*. **2009**, 150, 16-21. [5] H. Abe, Y. Imai, T. Takekiyo, Y. Yoshimura, *J. Phys. Chem. B* **2010**, *114*, 2834-2839. [6] Y. Yoshimura, T. Goto, H. Abe, Y. Imai, *J. Phys. Chem. B* **2009**, *113*, 8091-8095. [7] Y. Imai, H. Abe, T. Miyashita, T. Goto, H. Matsumoto, Y. Yoshimura, *Chem. Phys. Lett.* **2010**, 486, 37-39. [8] Y. Imai, H. Abe, H. Matsumoto, O. Shimada, T. Hanasaki, Y. Yoshimura, *J. Chem. Thermo.* **2011**, *43*, 319-322. [9] Y. Yoshimura, H. Kimura, C. Okamoto, T. Miyashita, Y. Imai, H. Abe, *J. Chem. Thermo.* **2011**, *43*, 410-412. [10] M. Aono, Y. Imai, Y. Ogata, H. Abe, T. Goto, Y. Yoshimura, T. Takekiyo, H. Matsumoto, T. Arai, *Metal. Mater. Trans. A*, **2011**, *42*, 37-40.

Keywords: Hierarchal Structure, Hydrogen bonding, H/D effect

MS30.P16

Acta Cryst. (2011) A**67,** C420

Interpretation and analysis of diffuse scattering using Monte Carlo simulation

Darren J. Goossens,[a,b] T.R. Welberry,[a] Aidan P. Heerdegen,[a] [a]*Research School of Chemistry, Australian National University, Canberra, (Australia).* [b]*Research School of Physics and Engineering, Australian National University, Canberra, (Australia).* E-mail: goossens@rsc.anu.edu.au.

Monte Carlo (MC) computer simulation of a model structure has become a powerful and well-accepted technique for aiding the interpretation and analysis of diffuse scattering patterns. The method consists of comparing diffraction patterns calculated from a computer model of the disordered structure with measured X-ray or neutron diffuse intensities. The advantage of the method is that it can be applied generally to all systems regardless of their complexity or the size of the atomic displacements that might be present. The only limitation is the extent to which the MC energy can be made to realistically represent the real system energy. At one extreme a very simplified model may be useful in demonstrating particular qualitative effects while at the other a quantitative and very detailed description of disordered structures can be obtained.

Over the last two decades the methodology has developed and improved enormously as a direct consequence of the (Moore's Law) increase in the power of computers (a factor of 10^6). In early studies [1], two-dimensional (2D) models representing projections of a crystal structure were used, simulations could only be carried out for a limited number of MC cycles and only qualitative comparisons were made between the model and the observed data. Now it is possible to use fully 3D models of a sufficient size to allow good representation of statistical properties, sufficient MC cycles to ensure that equilibrium distributions are attained and realistic interatomic or intermolecular potentials. The result is that models can be developed that give truly quantitative fits to observed diffuse scattering data and this allows detailed understanding of the mechanisms leading to the diffuse scattering [2].

In this paper we describe the advances that have been made and illustrate the progress using a variety of examples. These range from the different polymorphic forms of the pharmaceuticals benzocaine and aspirin, the flexible molecular compound *p*-(*N*-chlorobenzylidene)-*p*-chloroaniline, to a particularly interesting 19kDa viral protein example that exhibits frustration on a 73Å ×73Å triangular lattice.

[1]. T.R. Welberry, R.L. Withers, *Physics and Chemistry of Minerals* **1990,** *17*, 117-24. [2]. E.J. Chan *et al.*, *Acta Crystallographica Section B-Structural Science* **2009,** *65*, 382-92**.**

Keywords: diffuse scattering, monte-carlo, pharmaceuticals, viral protein.

MS30.P17

Acta Cryst. (2011) A**67,** C420

3D-PDF analysis of diffuse scattering from manganese Prussian Blue analog

Arkadiy Simonov,[a] Thomas Weber,[a] Walter Steurer,[a] Dmitry Chernyshov,[b] [a]*Laboratory of crystallography ETH Zürich (Switzerland)* [b]*Swiss-Norwegian Beam Line at the European Synchrotron Radiation Facility Grenoble (France).* E-mail: arkadiy.simonov@mat.ethz.ch

The metal substitutes of Prussian Blue are actively investigated because of their unique combination of magnetic and optical properties. All crystals in this family are disordered and disorder plays an important role for local physical properties like, for example, charge transfer. Information about the average structure alone is not sufficient for an understanding of such properties. By the use of X-ray diffuse scattering it is possible to obtain quantitative occupation correlations of disordered positions and accurate distances between atoms. Using this information one may build fragments of the real structure for modeling of physical properties.

In this work we present the results of direct three dimensional pair distribution function (3D-PDF) refinements of diffuse scattering from the manganese analog of Prussian Blue. The diffuse scattering was measured at the Swiss-Norwegian beam line at ESRF Grenoble. Qualitative analysis of the PDF showed presence of strong substitutional correlations and associated atomic displacements (the so called size effect). Direct 3D-PDF fitting is capable of refining all relevant correlation parameters. Explicit construction of a physical model is not required as it would be in case of the Monte Carlo refinements.

Keywords: diffuse, disorder, 3D-PDF

MS30.P18

Acta Cryst. (2011) A**67,** C420-C421

Modeling diffuse scattering on supercomputers with ZODS

Michal Chodkiewicza,[a] Hans-Beat Bürgi,[a] Thomas Weber,[b] Vickie Lynch,[c] Tara Michels-Clark,[c,d] [a]*Institute of Organic Chemistry, University of Zürich (Switzerland).* [b]*Laboratory of Crystallography, ETH Zürich (Switzerland),* [c]*Oak Ridge National Laboratory (USA),* [d]*University of Tennessee (USA).* E-mail: michalc@oci.uzh.ch

Single crystal structure determination from Bragg diffraction has become a largely routine operation. The information obtained is limited, however: it is the average over time and space of all crystallographic