

contribution we introduce a program that is aimed to be a swiss army knife for processing 3D-PDF and corresponding diffuse scattering data. Refinement tools are not included in this program and will be discussed elsewhere [4].

The features of the program currently include:

- quick and easy navigation through large 3D volumes,
- voxel precise editing of 3D data sets that may contain even more than one billion data points,
- separation of Bragg, diffuse and background scattering,
- symmetry averaging,
- transformation between reciprocal space and 3D-PDF space,
- tools that allow establishing a disorder model from 3D-PDF data.

To fulfill the requirements visualization of the data is done by pixel based imaging of 2D cuts through 3D data volumes instead of using iso-surface representations. Currently, the program supports its own format and the XCAVATE [5] file format, but other formats will be included if required. The program is by no means restricted to visualization and manipulation of 3D-PDF data, but may be used as a general editor for diffuse scattering data.

- [1] Schaub P., Weber T., Steurer W., *Philos. Mag.*, 2007, 87, 2781. [2] Kobas M., Weber T., Steurer W., *Phys. Rev. B* 2005, 71, 224205. [3] Schaub P., Weber T., Steurer W., *in preparation*. [4] Simonov A., Weber T., Steurer W., *in preparation*. [5] Estermann M., Steurer W., *Phase Trans.*, 1998, 67, 165.

Keywords: pair distribution function, diffuse scattering, data processing software

FA3-MS22-P12

Computer Simulation of Diffuse Scattering in Fe(II) Spin Crossover Compounds. M.Zubko^a, R.Neder^b, J.Kusz^a, P.Zajdel^a. ^a*Institute of Physics, University of Silesia, Poland.* ^b*Institute of Condensed Matter Physics, University of Erlangen-Nürnberg, Germany.*

E-mail: mzubko@us.edu.pl

Many Fe (II) spin crossover compounds show a thermal transition from the ¹A_{1g} low spin (LS) ground state to the excited ⁵T_{2g} high spin (HS) state. As a consequence the metal-ligand bond lengths increase by up to 0.2Å [1]. This increase has a strong impact on the whole crystal lattice as observed from the large temperature variation of the lattice parameters in the spin crossover region.

The compound [Fe(ptz)₆](BF₄)₂ (ptz=1-propyltetrazole) belongs to the group of the octahedrally coordinated Fe(II) spin crossover compounds. It crystallizes in space group R-3 (Z = 3) and the structure consists of exactly trigonal, neutral layers perpendicular to the c axis [2,3]. The iron atoms occupy special position 3(a) and all six ligands are equivalent. The (BF₄)⁻ anions are placed on the threefold axis.

Slow cooling through T_{1/2} = 123K causes appearance of diffuse scattering along the c* direction and splits Bragg peaks into two maxima. This indicates the presence of short range order in the low temperature diffuse phase [4].

Simulations and refinement of the disordered phase have been done with the DISCUS program package [5,6]. The simplest applied model consist of stacks of identical layers, which are stacked by either the perfect [1/3, -1/3, 1/3] vector or with an additional shift of [1/3+δ_x, -1/3+δ_y, 1/3]. The model is characterized by three parameters describing: the additional shift between neighbouring layers, the percentage of additionally shifted layers and the correlations along the c axis between shifted layers. The refinement of the parameters was

done through the differential evolutionary algorithm implemented in the DISCUS software package.

Computer simulations of X-ray diffuse scattering give insight into the real structure of the disordered phase of [Fe(ptz)₆](BF₄)₂ compound. The change of the peak shape with time and temperature can be explained by formation of lamellar domains perpendicular to the c direction. Such deformation becomes possible due to decrease of the interlayer Van der Waals forces caused by spin-crossover transition.

- [1] P.Gütlich, A.Hauser, H.Spiering, *Angew Chem Int Ed* 33(1994),2024. [2] P.L.Franke, Thesis, Rijks University, Leiden, 1982. [3] J. Kusz, H. Spiering, P. Gütlich, *J. Appl. Cryst.* 33(2004), 589. [4] J. Kusz, P. Gütlich, H. Spiering, *Top Curr. Chem.* 234(2004), 129. [5] Th. Proffen, R.B. Neder, *J. Appl. Cryst.* 30(1997), 171. [6] R.B. Neder, Th. Proffen, *Diffuse Scattering and Defect Structure Simulation*, Oxford University Press, 2008.

Keywords: diffuse X-ray scattering, disordered molecular crystals, computer simulation

FA3-MS22-P13

The Debye scattering formula in n dimensions

Thomas Wieder

E-mail: thomas.wieder@t-online.de

Consider an Euclidian coordinate system E_n of dimension $n = 1, 2, 3, \dots$. Let $r_{i,j}$ denote the interatomic distance vector among atoms i and j in an atomic assembly of M atoms within E_n . The contribution of $r_{i,j}$ to a diffraction pattern is obtained from an integration over the n -dimensional sphere of radius $|r_{i,j}| = r_{i,j}$. One arrives at the Debye scattering formula $I(k, n)$ valid in E_n . With k as the length of the scattering vector and with $f(k, i)$ as the atomic form factor the n -dimensional Debye scattering formula is

$$I(k, n) = \sum_{i=1}^M \sum_{j=1}^M f(k, i) f^*(k, j) F(k, n) \quad (1)$$

where one has

$$F(k, n) = 2^{\frac{n-1}{2}} \Gamma\left(\frac{n}{2}\right) (k r_{i,j})^{-\frac{n}{2}} \left(J\left(\frac{n}{2}, k r_{i,j}\right) n - J\left(\frac{n}{2} + 1, k r_{i,j}\right) k r_{i,j} \right)$$

with $\Gamma(x)$ as the Gamma function and $J(l, x)$ as the l -th Bessel function of the first kind.

For a given dimension n the formula (1) takes on a concrete form and such forms will be given for $n=2, \dots, 8$.

However, an application for cases with $n > 3$ is not known yet.

Keywords: scattering theory, amorphous scattering, analysis of disordered structures