

They include energy terms (for Monte-Carlo and other energy based simulations), joint probabilities (in crystal growth models) and parameters accounting for local distortions from the average structure. Models are constrained to show the symmetry of the average structure and of the observed diffuse scattering. Usage of a-priori chemical or structural knowledge is extensively supported. Various tools for analysis of the simulated crystals are provided.

As this type of calculations is known to be computationally demanding, especially if a global optimization of the parameters is performed, the software is targeted for use with supercomputers.

**Keywords: diffuse scattering, software design, supercomputing**

### FA3-MS22-P09

**The phase transition in the  $(\text{NbSe}_4)_{10/3}\text{I}$  charge-density-wave system.** J.Kusz<sup>a</sup>, M.Zubko<sup>a</sup>, A.Prodan<sup>b</sup>, H.J.P. van Midden<sup>b</sup>, J.C.Bennett<sup>c</sup>, H.Böhm<sup>d</sup>. <sup>a</sup>*Institute of Physics, University of Silesia, Katowice, Poland.* <sup>b</sup>*Jožef Stefan Institute, Ljubljana, Slovenia.* <sup>c</sup>*Department of Physics, Acadia University, Wolfville, Canada.* <sup>d</sup>*Institut für Geowissenschaften, University of Mainz, Germany*  
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$(\text{NbSe}_4)_{10/3}\text{I}$  belongs to the  $(\text{MX}_4)_n\text{Y}$  family of linear chain compounds. At room temperature it is a semimetal which changes at lower temperatures into a semiconductor [1]. The compound shows nonlinear transport properties with a charge density wave transition at 285K. A transmission electron microscopic study confirmed that the transition is of the Peierls type [2]. Single crystals of  $(\text{NbSe}_4)_{10/3}\text{I}$  were grown from the elements by means of a transport reaction in a two-zone furnace. The Xcalibur four-circle diffractometer (Oxford Diffraction) was used for data collections in the temperature range 80-300 K. A reversible transformation from a tetragonal into a monoclinic lattice with a domain structure was observed on cooling through the Peierls transition.

Single crystal X-ray analysis performed at room temperature confirms that the structure of  $(\text{NbSe}_4)_{10/3}\text{I}$  belongs to the space group  $P4/mcc$  with cell parameters  $a = 0.9464$  nm and  $c = 3.1906$  nm. Its one-dimensional nature is characterized by  $\text{NbSe}_4$  chains, aligned along the  $c$  axis. The niobium atoms are coordinated by Se antiprisms, stacked along the  $c$  axis in a screw-like arrangement. In accord with literature [3] the iodine atoms were found in two types of channels. In the first, running along the  $[00z]$  direction, four iodine atoms are closely bonded to four selenium atoms, while in the channels along the  $[\frac{1}{2}\frac{1}{2}z]$  direction only two iodine atoms are weakly bonded to eight selenium atoms in a square antiprismatic arrangement.

A weak diffuse scattering is detected perpendicular to the  $c^*$  direction in the entire temperature range examined. It is an indication of a short range order, which is present in both high and low temperature phases. Simulations of the disorder were performed with the DIFFUSE program package [4, 5], giving an insight into the real structure of  $(\text{NbSe}_4)_{10/3}\text{I}$ .

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171. [5] R.B.Neder, Th.Proffen, *Difuse Scattering and Defect Structure Simulation*, Oxford University Press, 2008.

**Keywords: charge density waves, diffuse X-ray scattering, one-dimensional conductors**

### FA3-MS22-P10

**Undulation fluctuations in the smectic A phase of goethite nanorods.** A.V. Petukhov<sup>a</sup>, E. van den Pol<sup>a</sup>, D.V. Byelov<sup>a</sup>, D.M.E. Thies-Weesie<sup>a</sup>, G.J. Vroege<sup>a</sup>.

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Anisometric (i.e., very non-spherical) colloidal particles are able to form liquid crystals, just like rod-like or disc-like molecules do. Here the application of microradian x-ray diffraction to characterize the structure of the smectic phase formed in the suspensions of goethite  $[\alpha\text{-FeOOH}]$  particles (average size  $280 \times 70 \times 30$  nm) will be described [1,2]. In particular, an unusual shape of the smectic reflections was observed with strong diffuse 'streaks' in the direction along the smectic layers [3]. This unusual peak shape is rationalized in terms of *sliding* fluctuations, in which the particle director stays fixed while the layers undulate by sliding the particles along each other. This undulation mode is different from the usually considered *splay* layer undulations, in which the nematic director follows the fluctuations of the layer normal. While the *splay* undulations destroy the long-range positional (Landau-Peierls instability), we show that the *sliding* fluctuations do not. Diffuse x-ray scattering tails around the smectic Bragg reflections allow one to distinguish which type of the fluctuations is dominant.

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### FA3-MS22-P11

**PDFView - A Program for Processing 3D Pair Distribution Function Data.** Thomas Weber.

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The three-dimensional pair distribution function method (3D-PDF) provides a direct access to information about disorder in crystals based on diffuse scattering data. It could be shown that this method allows qualitative and quantitative modeling of disorder in periodic crystals [1] as well as in quasicrystals [2, 3]. Though straightforward from a conceptual point of view, 3D-PDF investigations are currently time consuming and cumbersome tasks, because standard tools for data processing and refinement are not yet available. In this

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.

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**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<sup>a</sup>, R.Neder<sup>b</sup>, J.Kusz<sup>a</sup>, P.Zajdel<sup>a</sup>. <sup>a</sup>*Institute of Physics, University of Silesia, Poland.* <sup>b</sup>*Institute of Condensed Matter Physics, University of Erlangen-Nürnberg, Germany.*

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Many Fe (II) spin crossover compounds show a thermal transition from the <sup>1</sup>A<sub>1g</sub> low spin (LS) ground state to the excited <sup>5</sup>T<sub>2g</sub> 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)<sub>6</sub>](BF<sub>4</sub>)<sub>2</sub> (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 (BF<sub>4</sub>)<sup>-</sup> anions are placed on the threefold axis.

Slow cooling through T<sub>1/2</sub> = 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<sub>x</sub>, -1/3+δ<sub>y</sub>, 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)<sub>6</sub>](BF<sub>4</sub>)<sub>2</sub> 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.

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

### FA3-MS22-P13

**The Debye scattering formula in n dimensions**

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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**