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 $(NbSe_4)_{10/3}I$ charge-density-wave system. J.Kusz[a], M.Zubko[a], A.Prodan[b], H.J.P. van Midden[b], J.C.Bennett[c], H.Böhm[d]. [a]*Institute of Physics, University of Silesia, Katowice, Poland.* [b]*Jožef Stefan Institute, Ljubljana, Slovenia.* [c]*Department of Physics, Acadia University, Wolfville, Canada.* [d]*Institut für Geowissenschaften, University of Mainz, Germany*
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$(NbSe_4)_{10/3}I$ belongs to the $(MX_4)_nY$ 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 $(NbSe_4)_{10/3}I$ 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 $(NbSe_4)_{10/3}I$ 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 $NbSe_4$ 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 [½½z] 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 $(NbSe_4)_{10/3}I$.

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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[a], E. van den Pol[a], D.V. Byelov[a], D.M.E. Thies-Weesie[a], G.J. Vroege[a]. [a]*van 't Hoff laboratory for physical and colloid chemistry, Debye Institute for Nanomaterials Science, Utrecht University, The Netherlands.*
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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 [α-FeOOH] particles (average size 280×70×30 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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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