MS34-01 **Barium-IVc: A truly complex elemental crystal structure.** Ingo Loa, *The University of Edinburgh, United Kingdom*
E-mail: I.Loa@ed.ac.uk

Over the past decade, numerous elements have been observed to have high-pressure phases with complex crystal structures. These structures include incommensurate host-guest composite structures, incommensurately modulated structures and commensurate structures with large numbers of atoms in their unit cells. After a brief review of these phases, I will report the structural solution of a high-pressure phase of barium that takes the notion of structural complexity in the elements to a completely new level. This phase, barium-IVc, has been known for some time to exist at a pressure above ~17 GPa, but its powder diffraction pattern was too complex to interpret [1]. We have now studied this phase in detail by single-crystal synchrotron x-ray diffraction. The diffraction patterns are characterised by an unusual combination of sharp and diffuse reflections. Initial attempts to solve the structure using direct methods failed. I will show how the crystal structure was determined using a series of structural models with increasing detail and complexity. Barium-IVc has a host-guest composite structure with broken translational symmetry and a "basic unit" containing 768 atoms. The relative alignment of the guest-atom chains can be represented as a two-dimensional pattern with interlocking S-shaped 12-chain motifs repeating regularly in one direction and repeating with constrained disorder in the other.

[1] Nelmes R. J., *et al.*, Phys. Rev. Lett. **83**, 4081 (1999) and Proceedings of 17th AIRAPT, 475-8 (2000).

Keywords: crystal structure solution; high pressure; X-ray single-crystal diffraction

MS34-02 **Accessing disorder in single crystals by means of 3D-PDF analysis.** Arkadiy Simonov, Thomas Weber, Walter Steurer, *Laboratory of crystallography, ETH Zürich*
E-mail: arkadiy.simonov@mat.ethz.ch

X-ray diffuse scattering is a unique tool for analysis of disordered single crystals. Currently the most widely used method of the diffuse scattering interpretation is a Monte Carlo modeling. Despite the fact that it gives enormous flexibility in the construction of disordered crystals, refinement of diffuse scattering with MC technique is usually complicated. The main complication is due to the fact that refinement of Monte Carlo parameters is computationally demanding.

In this contribution we present a new method for diffuse scattering interpretation. The method is based on direct fitting of three-dimensional difference pair distribution function (3D-ΔPDF) of the crystal. The 3D-ΔPDF is the Fourier transform of diffuse scattering from a single crystal. It contains the information about interactions of pairs of atoms, ignoring the atoms, which are perfectly ordered as well fully uncorrelated atom pairs. When the average structure of a crystal is known, 3D-ΔPDFs can be easily interpreted qualitatively, and by PDF fitting one can obtain quantitative information about local structure correlations.

The application of the method is demonstrated on a solution of diffuse scattering from a real crystal. We also describe the impact of experimental problems like resolution function and background on the final result of diffuse scattering interpretation. These effects do not uniquely apply to the results of PDF refinements, but should be considered for the interpretation of diffuse scattering with any method.

Keywords: 3D-PDF; disorder; diffuse scattering