

Poster Presentation

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Precession Electron Diffraction studies of the phase transition in the (NbSe₄)₃I

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(NbSe₄)₃I is at room-temperature (RT) a semimetal, which changes at lower temperatures into a semiconductor [1]. The compound shows nonlinear transport properties with a second order phase transition at 274 K [2]. The symmetry of the RT (NbSe₄)₃I belongs to the P4/mnc space group and the structure is formed of NbSe₄ antiprisms, stacked along the c axis. The Nb atoms are grouped into Nb₂ segments and the Se-Se distances are correlated with the Nb chains. The I atoms occupy two types of channels; those running along the [00z] direction contain two I atoms connected to four Se atoms, while the channels along the [$\frac{1}{2}\frac{1}{2}z$] direction host two I atoms connected to eight Se atoms in a square anti-prismatic arrangement. At the (h,k, $\pm 6n$) planes a relatively strong diffuse scattering is present in the form of concentric rings. This scattering is explained by a similar model to the one recently suggested for (NbSe₄)₁₀/3I. The model is based on a mismatch between infinite NbSe₄ chains, randomly shifted along the c direction. (NbSe₄)₃I was studied by means of X-ray and electron diffraction with beam precession (PED) [3]. PED patterns usually contain more Bragg peaks than the conventional selected area diffraction patterns, because the intensity of the diffracted beams is integrated over the selected volume of the reciprocal space. An additional advantage of using the beam precession technique is a reduction of the dynamical interactions. Electron diffraction patterns were recorded sequentially, while tilting the crystal around an arbitrary crystallographic axis. Such space tomography allows a three-dimensional inspection of the reciprocal space and a more precise investigation of the diffuse scattering from nano-areas.

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