A Novel High-Pressure Tin Oxynitride Sn_2N_2O

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The crystal structure of a novel high pressure, high temperature tin oxynitride phase (Sn_2N_2O) was solved via Automated Electron Diffraction Tomography (ADT) [1]. The new phase was synthesized from a Sn-N-O precursor at 20 GPa and 1200-1500°C. Due to strong overlaps of symmetrically non-equivalent reflections, attempts to solve the unknown structure based on X-ray powder diffraction data were not successful. The use of the ADT method allows to collect three-dimensional electron diffraction data (3D ED) from single nanocrystals in the TEM via a tilt movement of the crystal and sequential diffraction pattern acquisition [2]. Subsequently, the reciprocal space is reconstructed and unit cell parameters as well as space group information can be derived. The electron diffraction intensities can be extracted and used to solve the crystal structure via approaches like “direct methods”.

The new oxynitride phase crystallizes in space group Pbcn with the unit cell parameters: a=7.83 Å, b=5.53 Å, c=5.54 Å. The crystal structure could be solved ab initio with direct methods and refined taking both the kinematic and dynamic theory of scattering into account. It resembles a Rh_2S_3 type structure where the Sn atoms are sixfold coordinated by O and N atoms. The refined structure compares very well with DFT calculations demonstrating the quality of data achievable with ADT and its applicability for the structure solution of high pressure and high temperature materials.

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Keywords: electron diffraction; high pressure materials; 3D ED; structure solution; synchrotron radiation