Structural phase transitions and the EoS of SnSe and SnTe at pressures up to 2 Mbar

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Tin telluride (SnTe) and tin selenide (SnSe) are narrow gap semiconductors with the properties of topological insulators [1,2] and pronounced thermoelectric effect [3,4]. These compounds undergo a variety of structural, electronic and topological changes at variations of pressure and temperature conditions [5].

In this work we studied high-pressure phase transitions in SnTe and SnSe in DAC using synchrotron XRD in a wide pressure range up to 2 Mbar and calculated equations of state (EoS) of these compounds [6,7].

SnSe: The structural properties of polycrystalline SnSe under conditions of ultrahigh pressures up to 205 GPa have been studied. Two structural phase transitions were found at $P \approx 2.5$ and ≈ 32 GPa. The first transition starts at 2.5 GPa and is accompanied by the continuous transformation of the orthorhombic GeS-type structure (sp.gr. *Pbnm*) into the structure of the Tl-type (sp.gr. *Cmcm*). In the pressure range 2.5–32 GPa, the two orthorhombic structures *Pbnm* and *Cmcm* coexist simultaneously. The second transition, at 32 GPa, corresponds to the transformation into a cubic structure of the CsCl-type ($Pm\bar{3}m$). In this case, an abrupt decrease in the unit cell volume occurs by about 7%. At pressures above 32 GPa, no new structural transitions were detected.

SnTe: Synchrotron X-ray diffraction studies of the SnTe structure at room temperature and pressures up to 193.5 GPa, created in DAC, have been carried out. Two structural phase transitions were found at pressures of 3 and 23 GPa. The first transition with an abrupt decrease in the unit cell volume by 4% is a result of the orthorhombic distortion of the initial cubic NaCl-type structure of SnTe-B1. In the pressure range of $3 < P < 23$ GPa, the region of coexistence of two intermediate orthorhombic phases SnTe with space groups *Cmcm* and *Pnma* was established. At a pressure of ~ 23 GPa, a second phase transition from the intermediate orthorhombic modifications to the cubic phase SnTe-B2 with the structural type CsCl was detected. This is the first-order transition and it is accompanied by an abrupt decrease in the volume cell by 8%. In the pressure range of 23–193.5 GPa, no additional phase transitions were detected.

The pressure dependences of the specific volume of the unit cells at room temperature and Birch-Murnaghan EoS for SnSe and SnTe are shown in Fig. 1 and Fig. 2 respectively.

The results of this study are critical for understanding the electronic and structural properties of SnSe and SnTe, as well as for more accurate theoretical calculations and predictions of the properties of these compounds including the search for a possible superconducting state.

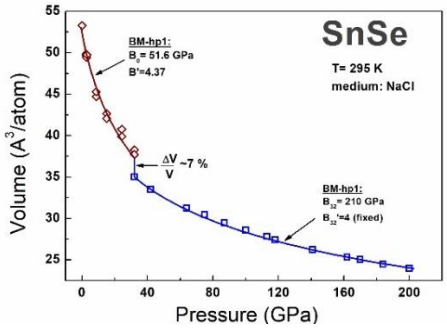

Figure 1. Equation of state SnSe up to 203 GPa

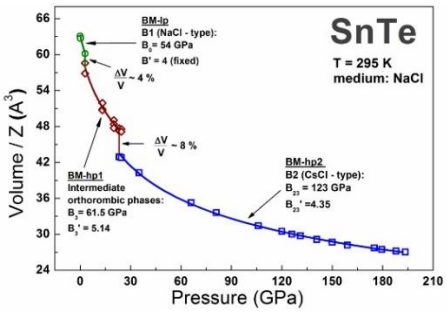

Figure 2. Equation of state for SnTe up to 193 GPa

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