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Structural Phase Transitions and the Equation of State in SnSe at High Pressures up to 2 Mbar

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The crystal structure of tin selenide SnSe has been studied under quasihydrostatic compression at pressures up to 205 GPa created in diamond anvil cells at room temperature. Two structural phase transitions have been detected at $P \approx 2.5$ and 32 GPa. The former phase transition is continuous from the GeS-type structure (space group *Pbnm*) to the TlI-type structure (space group *Cmcm*). The phase transition to the CsCl-type cubic structure (space group $Pm\bar{3}m$) occurs at 32 GPa and is accompanied by a stepwise decrease in the volume of the unit cell by 7%. The pressure dependence of the specific volume of the unit cell at room temperature has been constructed up to 205 GPa.

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1. INTRODUCTION

Tin selenide SnSe under ambient conditions is an indirect band gap semiconductor with a gap width in the range of 0.86–1 eV with a GeS layered orthorhombic structure (space group *Pbnm*). This compound has attracted great attention in recent times in view of an ultralow lattice thermal conductivity and a pronounced thermoelectric effect [1–3]. It has recently been established that thin films of metastable SnSe with a NaCl cubic structure obtained by epitaxy have the properties of a topological crystalline insulator [4, 5].

Under quasihydrostatic compression at pressures above 27 GPa, SnSe demonstrates superconductivity [6]. At this pressure, SnSe undergoes a structural phase transition to a CsCl-type phase (space group $Pm\bar{3}m$). With increasing pressure, the critical temperature of the superconducting phase transition T_c in this phase reaches a maximum of 3.2 K at a pressure of 39 GPa. The detection of superconductivity in SnSe with $T_c \sim 4.5$ K at pressures above 56 GPa was reported in 1997 [7]. Taking into account the known structural phase transitions in IV–IV compounds, the authors of [7] assumed that superconductivity in SnSe is observed in a phase with a CsCl-type structure. However, the structural properties of SnSe (and the existence of any structural phase transitions) at pressures above 55 GPa remain unclear.

To reveal mechanisms of superconductivity and the properties of the superconducting phase of SnSe, it is necessary to determine the crystal structure of SnSe in a wide pressure range. In this work, the crystal structure of tin selenide SnSe is studied under quasihydrostatic compression at pressures up to 205 GPa created in diamond anvil cells.

2. EXPERIMENTAL PROCEDURE

Polycrystalline SnSe samples were synthesized by the solid-phase reaction method. Initial components Sn and Se were mixed in a stoichiometric proportion and were placed in quartz glass ampoules. The ampoules were evacuated, sealed, and placed in a tube furnace. The temperature in the furnace was increased from 200 to 600°C at several stages for three weeks.