Zinc selenide (ZnSe) is an important luminescent semiconductor with a wide direct band gap. At ambient pressure and moderate temperatures, the thermodynamically stable phase is sphalerite ZnSe (F43m), while above 1698(2) K it transforms into hexagonal wurtzite polymorph (P63mc) [1,2] that congruently melts at 1795(2) K [2]. Similarly to many other II-VI compounds ZnSe undergoes pressure-induced phase transition from 4-fold coordination into dense rock-salt structure (Fm3m) with 6-fold coordination [1]. The equilibrium phase boundary between sphalerite and rock-salt ZnSe polymorphs was determined as $p$ (GPa) = $12.21 - 0.0039 \cdot T$ (ºC) [3].

Phase relations and melting of sphalerite ZnSe have been in situ studied up to 6 GPa and 2100 K using energy-dispersive synchrotron X-ray diffraction and multianvil high-pressure systems MAX80 (beamline F2.1) and MAX200x (beamline W2) of the DORIS III storage ring.

Above 1 GPa formation of wurtzite ZnSe is completely suppressed which should allow growing high quality single crystals of sphalerite ZnSe by crystallization from the melt. From 1 to 6 GPa sphalerite ZnSe is the only thermodynamically stable polymorph up to the melting. Its phase transition into dense rock-salt phase reported earlier [3] has not been observed in the whole pressure–temperature range under study. The slope of ZnSe melting curve is 45(5) K/GPa.

Phase $p$-$T$ diagram of ZnSe. The black circles correspond to solid sphalerite ZnSe, while the open ones to completely molten. Solid red line shows the melting curve of ZnSe (present work); dashed blue line shows the solid-solid phase boundary according to Kusaba & Kikegawa [3]. The open squares and triangles correspond to rock-salt and sphalerite ZnSe, respectively.

References