



Pressure-Induced Phase Transitions in Cadmium Thiogallate CdGa₂Se₄

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Abstract

The high-pressure behavior of semiconducting cadmium thiogallate CdGa2Se4 with the defect chalcopyrite structure (I4, Z=2) is studied by in situ angle-dispersive synchrotron X-ray powder diffraction and optical reflectivity measurements in a diamond anvil cell at room temperature. At 21 GPa an order–disorder phase transition to the rock-salt structure (F43m, Z=4) occurs. Upon decompression, the metallic NaCl-type polymorph transforms into zinc-blende (Fm3m, Z=4) at pressures of 7.5–4 GPa. The recovered metastable semiconducting material is of the zinc-blende type.