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Phase transition and thermoelastic behavior of cadmium sulfide at high pressure and high temperature

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Abstract

The phase transition and thermal equation of state of cadmium sulfide (CdS) were studied at high pressure and temperature conditions up to 21.9 GPa and 650 K, by using *in situ* synchrotron angle-dispersive X-ray diffraction and an externally-heated diamond anvil cell (DAC). A pressure-induced phase transition from wurtzite structure (WZ) to rocksalt structure (RS) was observed at about 2.6 GPa, which was agreed with previous studies (2.0-3.5 GPa). In addition, fitting of the experimental data by means of the third-order Brich-Murnaghan equation of state (III-BM EoS) gives the bulk modulus K_0 = 81.6 (13) GPa, its pressure derivative K'_0 = 3.68 (13), and the volumetric thermal expansion coefficient α_0 = 2.97 (25) $\times 10^{-5}$ K^{-1} for RS phase of CdS. Simultaneously, the thermal expansion coefficient (α_0 =1.51$\times 10^{-5}$ K^{-1}), and its axial thermal expansivities (8.30$\times 10^{-6}$ K^{-1} and 5.96$\times 10^{-6}$ K^{-1}) along *a*-axis and *c*-axis for WZ phase of CdS at ambient conditions were obtained, respectively. Moreover, it was found that the phase transition pressure from WZ (or ZB) type to RS type of cadmium chalcogenides (CdS, CdSe and CdTe) is quite similar by comparing their phase transition pressures. Furthermore, the elastic properties of metal sulfides (ZnS, CdS, HgS, PbS) with the same crystal structure but different metal cations were also discussed, and found that the bulk moduli for the RS phase of metal sulfides (ZnS, CdS, HgS, PbS) have a negative correlation with the cation radius, but a positive correlation with the electronegativity.

Keyword

Cadmium sulfide (CdS); High temperature and high pressure; X-ray diffraction; *PVT* equation of state; Diamond anvil cell (DAC)