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

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1 **Phase transition and thermoelastic behavior of cadmium sulfide at**  
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12 **Abstract**

13 The phase transition and thermal equation of state of cadmium sulfide (CdS) were  
14 studied at high pressure and temperature conditions up to 21.9 GPa and 650 K, by  
15 using *in situ* synchrotron angle-dispersive X-ray diffraction and an externally-heated  
16 diamond anvil cell (DAC). A pressure-induced phase transition from wurtzite  
17 structure (WZ) to rocksalt structure (RS) was observed at about 2.6 GPa, which was  
18 agreed with previous studies (2.0-3.5 GPa). In addition, fitting of the experimental  
19 data by means of the third-order Birch-Murnaghan equation of state (III-BM EoS)  
20 gives the bulk modulus  $K_0 = 81.6$  (13) GPa, its pressure derivative  $K'_0 = 3.68$  (13), and  
21 the volumetric thermal expansion coefficient  $\alpha_0 = 2.97$  (25)  $\times 10^{-5} \text{ K}^{-1}$  for RS phase of  
22 CdS. Simultaneously, the thermal expansion coefficient ( $\alpha_0 = 1.51 \times 10^{-5} \text{ K}^{-1}$ ), and its  
23 axial thermal expansivities ( $8.30 \times 10^{-6} \text{ K}^{-1}$  and  $5.96 \times 10^{-6} \text{ K}^{-1}$ ) along *a*-axis and *c*-axis  
24 for WZ phase of CdS at ambient conditions were obtained, respectively. Moreover, it  
25 was found that the phase transition pressure from WZ (or ZB) type to RS type of  
26 cadmium chalcogenides (CdS, CdSe and CdTe) is quite similar by comparing their  
27 phase transition pressures. Furthermore, the elastic properties of metal sulfides (ZnS,  
28 CdS, HgS, PbS) with the same crystal structure but different metal cations were also  
29 discussed, and found that the bulk moduli for the RS phase of metal sulfides (ZnS,  
30 CdS, HgS, PbS) have a negative correlation with the cation radius, but a positive  
31 correlation with the electronegativity.

32 **Keyword**

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

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