PCCP

PAPER

View Article Online
View Journal | View Issue

Phase transformation of cadmium sulfide under high temperature and high pressure conditions

Cite this: *Phys. Chem. Chem. Phys.*, 2014, **16**, 14899

Jianwei Xiao,[a] Bin Wen,*[a] Roderick Melnik,[b] Yoshiyuki Kawazoe[cd] and Xiangyi Zhang[a]

Received 8th March 2014,
Accepted 29th April 2014

DOI: 10.1039/c4cp01003e

www.rsc.org/pccp

Cadmium sulfide (CdS) is one of the most significant wide band gap semiconductors, and knowledge of the phase transformation of CdS under high temperature and pressure is especially important for its applications. The pressure–temperature phase diagram and the phase transformation pathways of CdS have been investigated by using density functional theory combined with quasiharmonic approximation. Our results indicated that under ambient conditions, wz-CdS is a stable phase, while under high temperature and pressure, rs-CdS becomes the stable phase. It is also found that zb-CdS is an intermediate phase in transforming from rs-CdS to wz-CdS. Therefore, although there are no zb-CdS phase regions in the CdS pressure–temperature phase diagram, zb-CdS can be found in some prepared experiments.

I. Introduction

Cadmium sulfide (CdS) is one of the most significant wide band gap ($\sim$2.4 eV) semiconductors with excellent optoelectronic properties. It has been widely used in the fields of infrared materials, photovoltaic cells, sensors, energy storage materials and photocatalysts.[1–5] CdS exists in three phases, including the wurtzite structure (wz-CdS) with a direct band gap of $\sim$2.4 eV,[1,5–7] the zinc-blende structure (zb-CdS) with a band gap of $\sim$2.55 eV,[8] and a high pressure rocksalt structure (rs-CdS) with an indirect band gap of $\sim$1.5 eV.[7,9] To maintain excellent optoelectronic properties, CdS must remain in the wurtzite structure for practical applications. Therefore, the structural phase transformation in CdS crystals becomes an important issue, and it has attracted many theoretical and experimental studies. By comparing the enthalpy of wz-CdS, zb-CdS and rs-CdS, Tan *et al.* found that wz-CdS and zb-CdS can be transformed into rs-CdS under high pressure conditions, and the critical transformation pressures are 2.6 and 2.57 GPa, respectively.[5] Similar results have been obtained by first principles calculations,[1] optical-absorption experiments,[9] Raman scattering,[10–12] and X-ray diffraction.[13] In reality, temperature plays an important role in the structural phase transformation processes,[14] thus the influence of temperature on the structural phase transformation of CdS crystals cannot be ignored. Although many experimental methods have already been developed to study the high temperature and high pressure (HTHP) phase transformation of materials, it is still difficult and expensive to perform HTHP phase transformation experiments on materials due to the complexity of sample preparation and the need to maintain the sample under HTHP conditions. Hence, no HTHP structural phase transformations and pressure and temperature (*P*–*T*) phase diagrams of CdS crystals have been studied systematically in previous works.[1,5,9–13] With ready availability of computing power, computational methods become an important alternative tool to study HTHP phase transformations of materials. Recently, density functional theory combined with quasiharmonic approximation theory (DFT-QHA)[15] has been developed for studying the structures and properties of crystals under HTHP conditions,[16] and it has been successfully used in many different crystal structures.[17–19] This method provides an effective tool for the study of structural phase transformation under HTHP conditions and further allows the construction of the *P*–*T* phase diagram of CdS crystals.

In this work, the structural phase transformation under HTHP conditions and the *P*–*T* phase diagram of CdS crystals have been studied by using DFT-QHA theory. Furthermore, the phase transformation pathways among these CdS crystals have also been investigated. Our results indicated that under ambient conditions, the wz-CdS is a stable phase; while under HTHP conditions, rs-CdS becomes the stable phase, and zb-CdS is the intermediate phase in the transformation from rs-CdS to wz-CdS.

---

[a] *State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China. E-mail: wenbin@ysu.edu.cn*
[b] *M^{2}NeT Lab, Wilfrid Laurier University, Waterloo, 75 University Ave. West, Ontario, Canada N2L 3C5*
[c] *New Industry Creation Hatchery Center, Tohoku University, 6-6-4 Aramaki-aza-Aoba, Aoba-ku, Sendai 980-8579, Japan*
[d] *Institute of Thermophysics, Siberian Branch of the Russian Academy of Sciences, 1, Lavyrentyev Avenue, Novosibirsk 630090, Russia*

II. Computational methods

According to the DFT-QHA method,[15] the Gibbs free energy at different pressures and temperatures $G(T,P)$ can be calculated by the following equation:

$$G(T,P) = F(T,V) + PV, \tag{1}$$

where $F(T,V)$ represents the Helmholtz free energy of the crystal. It is expressed as follows:

$$F(T,V) = E(V) + F_{\mathrm{ph}}(T,V). \tag{2}$$

In this equation, $E(V)$ denotes the total energy, and F_{ph} is the phonon vibration energy at a given volume V. Hence, $G(T,P)$ can be expressed as:

$$G(T,P) = E(V) + PV + F_{\mathrm{ph}}(T,V). \tag{3}$$

The total energy is obtained by using density functional theory (DFT) based on the plane-wave pseudopotential technique as implemented in the VASP package.[20] The exchange and correlation interactions have been described in the local density approximation (LDA-CAPZ).[21] The kinetic cutoff energy for plane waves was set as 600 eV. The k point separation in the Brillouin zone was $9 \times 9 \times 9$ for zb-CdS and rs-CdS, and $13 \times 13 \times 5$ for wz-CdS. The convergence energy and force are set to 1×10^{-6} eV per atom and 1×10^{-3} eV Å^{-1} with respect to electronic, ionic and unit cell degrees of freedom. The LDA method has been used in this work, since it can give reasonable lattice constants of wz-CdS and rs-CdS in comparison with GGA.[1] In addition, our benchmark calculations are conducted for the rs-CdS phase; the calculated lattice constant a = 5.355 Å agrees well with the experimental value of a = 5.44 Å.[22] Meanwhile, the lattice parameters for wz-CdS are a = 4.088 Å and c = 6.662 Å; they are in good agreement with the experimental values of a = 4.136 Å and c = 6.714 Å.[23] These results confirmed that our present computational scheme is reliable.

The phonon vibration energy $F_{\mathrm{ph}}(T,V)$ can be described by the following equation:

$$F_{\mathrm{ph}}(T,V) = K_{\mathrm{B}}T\int_0^{\infty} g(w)\ln[2\sin(\hbar w/2k_{\mathrm{B}}T)]\mathrm{d}w, \tag{4}$$

where $\omega = \omega(V)$ represents the volume dependent phonon frequencies and $g(\omega)$ is the phonon density of state in a fixed volume. The phonon frequencies and the phonon density of state for a fixed volume are calculated by using the PHONOPY program.[24] This program used the force constants calculated from the optimized supercell, and the size of the supercell for the phonon calculations was set at $2 \times 2 \times 2$, which contains 32, 64 and 64 atoms for wz-CdS, zb-CdS and rs-CdS, respectively.

III. Results and discussion

A. Structural properties and phonon dispersion of wz-CdS, zb-CdS and rs-CdS

Three CdS polytypes (wz-CdS, zb-CdS and rs-CdS) have been built by using crystallographic data in ref. 5, and their cell parameters and atomic positions have been optimized under the pressure range of −6 to 6 GPa. As a result, the corresponding total energies $E(V)$ have been obtained, and are plotted in Fig. 1. The lattice constants, atom positions and the cohesive energy E_{coh} (fitted by using Murnaghan's equation of state structure[25]) of three CdS polytypes at 0 GPa along with experimental and previous theoretical data are summarized in Table 1. The optimized lattice parameters agree well with the previous theoretical and experimental results.[5,7,22,23,26,27] There is one type of bond for zb-CdS and rs-CdS, and the corresponding bond lengths are 2.501 and 2.677 Å, respectively. The bond length of rs-CdS is larger than that of zb-CdS, but the mass density of rs-CdS is larger than that of zb-CdS because the coordination number of rs-CdS (6) is larger than that of zb-CdS (4). The mass densities of wz-CdS and zb-CdS are similar due to their analogous bond lengths and coordination numbers. wz-CdS, with the lowest cohesive energy E_{coh} (−3.712 eV per atom), is the most stable phase at 0 GPa, and it also has the lowest total energy $E(V)$. The cohesive energy E_{coh} (−3.71 eV per atom) and total energy $E(V)$ values of zb-CdS are much closer to those of wz-CdS.

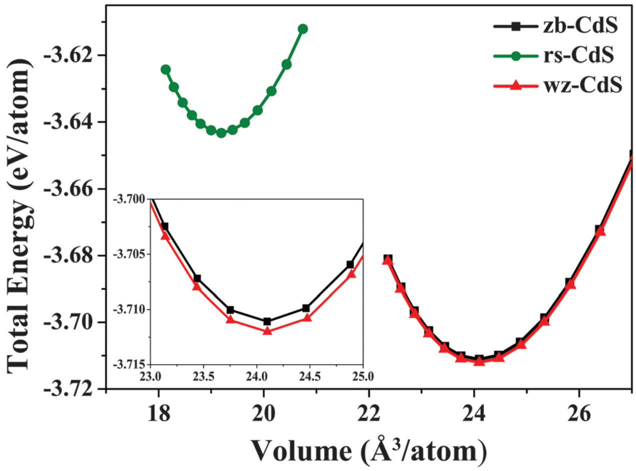

Fig. 1 The calculated total energy $E(V)$ of wz-CdS, zb-CdS and rs-CdS. The inset figure shows an enlarged section of the $E(V)$ curves of wz-CdS and zb-CdS.

To study the dynamical stability of CdS phases, the phonon band structure along the high symmetry directions of the Brillouin zone and the phonon densities of state (DOS) for all three CdS phases have been calculated, and they are shown in Fig. 2. As can be seen, no imaginary frequencies exist at the vibration frequencies of rs-CdS, wz-CdS and zb-CdS at 0 GPa. Therefore, rs-CdS, wz-CdS and zb-CdS are dynamically stable phases at 0 GPa. It is noteworthy that wz-CdS has four atoms in its primitive unit cell, and there are twelve phonon branches in its phonon band structure (shown in Fig. 2a). Also, wz-CdS belongs to the $C_{6v}{}^{4}$ space group, and there exist A1 and E1 infrared modes at the Gamma point.[28] Furthermore, at the Gamma point these modes split into longitudinal and transverse (LO and TO) components due to the ionic character of the crystal,[5,28] and the LO–TO splitting causes the frequency of the LO optical mode to be higher than that of the TO optical mode. But for zb-CdS and rs-CdS, there are two atoms in their respective primitive unit cells, thus six phonon modes exist in their phonon band structures. The distinction is that a gap

Table 1 Optimized crystallographic data, bond length, mass density (D), and the cohesive energies E_{coh} for different cadmium sulfide polytypes at a pressure of 0 GPa

Phase	Space group	Lattice parameters (Å)	Atom position	Bond length (Å)	Coordinated	D (g cm^{-3})	E_{coh} (eV per atom)	Ref.
zb-CdS	$F\bar{4}3m$ (216)	a = 5.777	Cd (0 0 0)	2.501	4	4.98	−3.71	This work
		a = 5.776	S (1/4 1/4 1/4)					5
		a = 5.808						26
		a = 5.87						27
		a = 5.818						Expt. 23
wz-CdS	$P6_3mc$ (186)	a = 4.088, c = 6.662	Cd (1/3 2/3 0)	2.505	4	4.98	−3.712	This work
		a = 4.086, c = 6.667	S (1/3 2/3 3/8)	2.5				5
		a = 4.18, c = 6.76						7
		a = 4.19, c = 6.66						27
		a = 4.136, c = 6.714						Expt. 23
rs-CdS	$Fm\bar{3}m$ (225)	a = 5.355	Cd (0 0 0)	2.677	6	6.25	−3.656	This work
		a = 5.358	S (0 0 1/2)					5
		a = 5.3527						26
		a = 5.45						7
		a = 5.44						Expt. 22

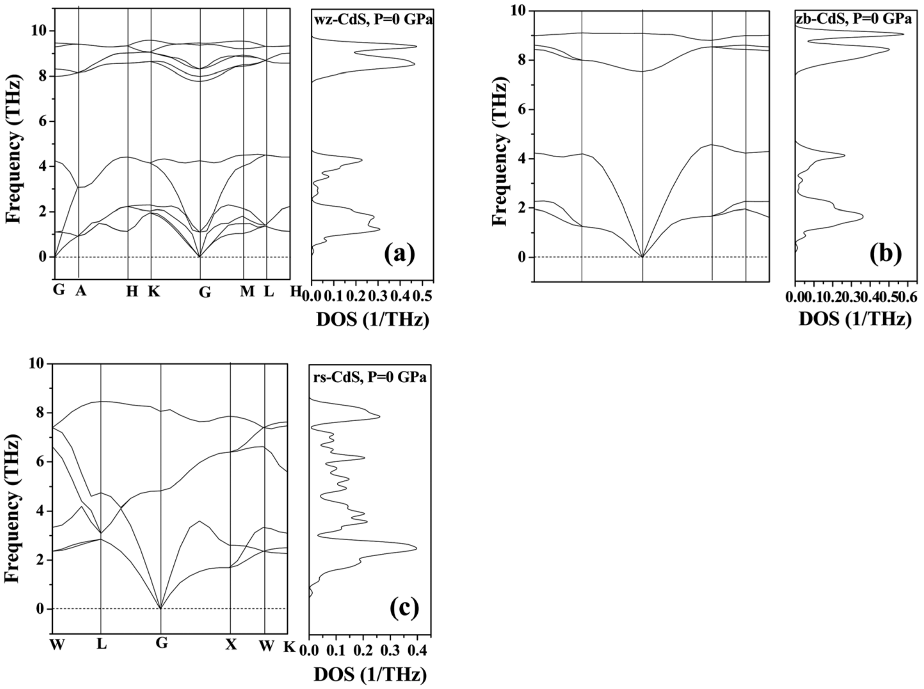

Fig. 2 The phonon band structure and the density of states (DOS) for wz-CdS (a), zb-CdS (b), and rs-CdS (c) at 0 GPa.

exists between optical modes and acoustic modes in the phonon dispersion of zb-CdS, but for rs-CdS, there is no such gap in its phonon band structure. Similar to wz-CdS, the LO-TO splitting at the Gamma point also exists in the phonon band structures of zb-CdS and rs-CdS (shown in Fig. 2b and c). By comparing the phonon data of wz-CdS and zb-CdS, we found that both have peaks at frequencies of 9 THz, 8 THz, 4 THz and 1.6 THz. This result indicated that the phonon properties of wz-CdS and zb-CdS are similar.

B. Phase diagram of cadmium sulfide

In this work, volume deformation was performed under constant hydrostatic pressure conditions. Furthermore, the volume thermal expansion of CdS crystals is not considered since the thermal expansion of lattice constants is very small.[29,30] To construct the P–T diagram of CdS, the phase with the lowest Gibbs free energy among the three CdS phases needs to be found under given pressure and temperature conditions. For example, the relative Gibbs free energies of wz-CdS and zb-CdS with respect to rs-CdS at a pressure of 0 GPa and temperatures ranging from 0 to 2000 K are plotted in Fig. 3a. The results indicated that the phase transformation temperatures are 1160 K from zb-CdS to rs-CdS, and 1235 K from wz-CdS to rs-CdS. Therefore, the lowest Gibbs free energy phase at this temperature and pressure can be found. In similar way, the phase with the lowest Gibbs free energy among the three CdS

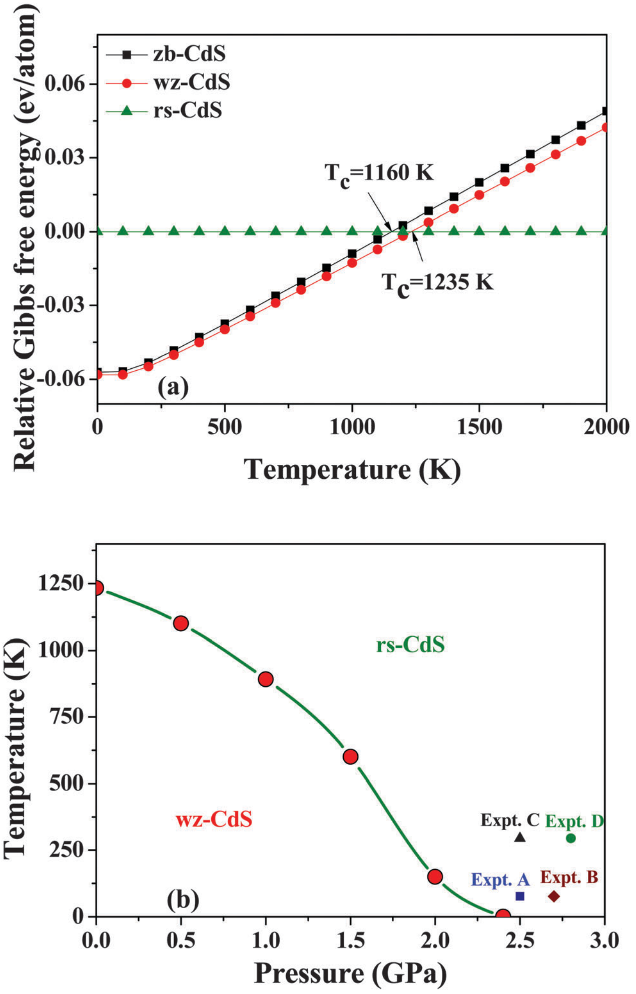

Fig. 3 (a) The relative Gibbs free energy *vs.* temperature for wz-CdS and zb-CdS with respect to rs-CdS at a pressure of 0 GPa. (b) The calculated P–T phase diagram for CdS compared with experimental points. A and B, Raman spectra (ref. 11 and 12); C, X-ray diffraction (ref. 13); D, optical-absorption experiment (ref. 9).

phases at different pressure and temperature conditions has been calculated correspondingly, and the P–T phase diagram of CdS is constructed, as presented in Fig. 3b. It reflects that at lower temperature and pressure regions, wz-CdS is a stable phase, while at higher temperature and pressure regions, rs-CdS becomes the stable phase. Furthermore, the phase transformation pressure is 2.4 GPa from wz-CdS to rs-CdS at 0 K, and the phase transformation temperature is 1235 K from wz-CdS to rs-CdS at 0 GPa. The results of our investigations agree well with the previous experimental and theoretical data,[1,5,9–13] even though the long wavelength phonons have been ignored in the phonon frequencies computational process.[15] Owing to the similarity of phonon properties, the Gibbs free energies of zb-CdS and wz-CdS are very close, but the Gibbs free energy of zb-CdS is always higher than that of wz-CdS. Therefore, there is no zb-CdS phase region in the CdS P–T phase diagram. Nevertheless, under ambient conditions the zb-CdS phase can be found experimentally. To further understand why zb-CdS can exist under ambient conditions, the phase transformation pathways among wz-CdS, zb-CdS and rs-CdS have been investigated.

C. Phase transformation pathway among wz-CdS, zb-CdS and rs-CdS

To determine the phase transformation pathways among wz-CdS, zb-CdS and rs-CdS, a series of intermediate structures has been built by finding the common subgroups of space groups of these structures. This method has been successfully used to investigate the phase transformations for many crystals.[31–33] The high-symmetry common subgroups, for which the Wyckoff letter and site symmetry match, are considered the phase transformation pathway between reactant and product structures. It is known that the space groups of wz-CdS, zb-CdS and rs-CdS are $P6_3mc$ (No. 186), $F\bar{4}3m$ (No. 216), and $Fm\bar{3}m$ (No. 225), respectively. By comparison, for the subgroups of these crystal structures, as listed in the *International Tables for Crystallography*,[34] we found that $Pca2_1$ (No. 29) may serve as the space group of the intermediate structure in the structural phase transformation process from wz-CdS to zb-CdS, and also from wz-CdS to rs-CdS. For the structural phase transformation from zb-CdS to rs-CdS, the intermediate structure's space group is $Imm2$ (No. 44), and this space group has also been used to study the structural phase transformation from zinc-blende to rocksalt structures for other compounds.[35] Therefore, the intermediate structures in the transformation from zb-CdS to rs-CdS have an orthorhombic lattice with a space group of $Imm2$, and their unit cell includes two atoms with fractional coordinates of Cd (0, 0, 0) and S (0, 0.5, z), respectively. From wz-CdS to zb-CdS, the intermediate structures have an orthorhombic lattice with a space group of $Pca2_1$, and their unit cell includes four atoms with fractional coordinates of S1 ($-0.91667 - 0.333z$, $0.125 - 0.5z$, 0.5625), S2 ($-0.41667 - 1.333z$, $0.375 + 0.5z$, $0.5625 + z$), Cd1 ($-0.91667 - 1.333z$, $0.125 - 0.5z$, $0.9375 - z$) and Cd2 ($-0.41667 - 0.08333z$, $0.375 + 0.125z$, 0.9375), respectively. Similar to the phase transformation from wz-CdS to zb-CdS, the space group of the intermediate structure from wz-CdS to rs-CdS is also $Pca2_1$, and its unit cell includes four atoms with fractional coordinates of S1 ($0.58333 - 0.1667z$, $0.375 + 0.25z$, $0.9375 - 0.245z$), S2 ($0.08333 + 0.333z$, $0.125 - 0.25z$, $0.9375 - 0.75z$), Cd1 ($0.58333 - 0.667z$, $0.375 + 0.25z$, $0.5625 + 0.505z$,) and Cd2 ($0.08333 - 0.1667z$, $0.125 - 0.25z$, $0.5625 + 0.005z$). The z values ranging from 0 to 0.5 are regarded as the intermediate parameters. For z = 0, 0.25 and 0.5 the structures are wz-CdS, zb-CdS and rs-CdS, respectively. In this work, each intermediate structure has been fully relaxed at 0 GPa by fixing the fractional coordinates of atoms, and finally the enthalpies have been obtained, and they are plotted in Fig. 4.

As can be seen from Fig. 4, the energy barrier from rs-CdS to wz-CdS is about 3.4 eV per atom, and this energy barrier is so high that the phase transformation cannot happen along this transformation path under ambient conditions. But for the structural phase transformation from rs-CdS to zb-CdS, the energy barrier is about 0.1 eV per atom, and it is about 0.87 eV per atom from zb-CdS to wz-CdS. Therefore, the direct transformation from rs-CdS to wz-CdS is far less favorable than the

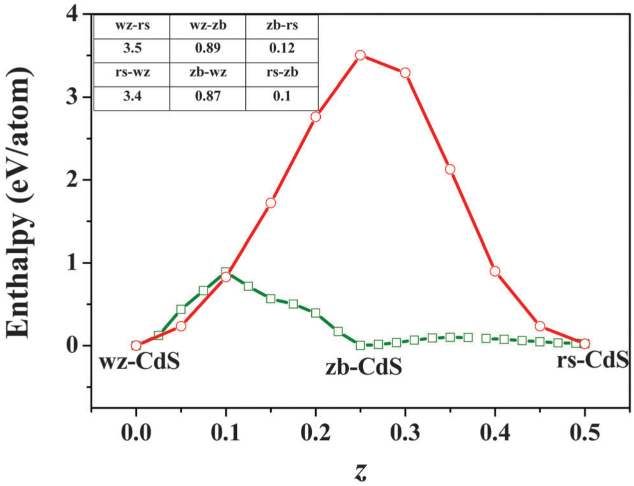

Fig. 4 Energy path from wz-CdS to rs-CdS, from zb-CdS to rs-CdS, and from wz-CdS to zb-CdS. The energy barrier is shown in the inset table.

indirect transformation with zb-CdS as the intermediate phase. These results suggested that zb-CdS may be an intermediate phase in the transformation from rs-CdS to wz-CdS. To further explore the possible intermediate phase from rs-CdS to wz-CdS, a crystal structure search for the candidate structure of CdS has been performed using the inorganic crystal structure database (ICSD).[36] In fact, this method has been widely used to determine the structures of different materials.[37,38] These found structures of CdS have been optimized, and their relative energies with respected to zb-CdS have been summarized in Table 2. The results indicated that under ambient conditions, the energy of the cubic $F\bar{4}3m$ (zb-CdS) structure is higher than that of the hexagonal $P6_3mc$ (wz-CdS) structure, and lower than that of the cubic $Fm\bar{3}m$ (rs-CdS) structure. Besides, the energy of other candidate structures of CdS is above the energy of rs-CdS.

Table 2 Energy of considered candidate structures of CdS with different space groups found from an ICSD search, given in eV per atoms, respected to the zb-CdS

Structure	Space group	Energy (eV per atom)
zb-CdS	$F\bar{4}3m$ (216)	0
ZnS	$P6_3mc$ (186)	−0.008
ZnS	$F\bar{4}3m$ (216)	0.0
NaCl	$Fm\bar{3}m$ (225)	0.057
InCl	$Ama2$ (40)	0.327
lnCl	$Ama2$ (40)	0.433
lnCl	$Cmcm$ (63)	0.374
lnCl	$Cmc2_1$ (36)	0.402
lnBi	$P4/nmm$ (129)	0.430
TaN	$P\bar{6}2m$ (189)	0.17
GaTe	$C2/m$ (12)	0.697
GaPt	$Pnma$ (62)	0.333
InSe	$R3m$ (160)	0.459
NS	$P2_1/c$ (14)	0.52
N4S4	$P2_1/c$ (14)	1.008
PtSi	$Pnma$ (62)	0.308
P4S4	$C2/m$ (12)	0.617
PdPu	$Pnma$ (62)	0.383
AlLi	$Fd\bar{3}m$ (227)	0.841
Aucl	$I4_1/amd$ (141)	0.61
Cscl	$Pm\bar{3}m$ (221)	0.617

These results demonstrate that zb-CdS is the intermediate phase in the structural phase transformation process from rs-CdS to wz-CdS. Therefore, although there are no zb-CdS phase regions in the CdS P–T phase diagram, zb-CdS or a mixture of zb-CdS and wz-CdS can be found in some prepared experiments.[3,39,40]

IV. Conclusion

By using density functional theory combined with a quasiharmonic approximation method, the high temperature and high pressure phase diagram and phase transformation pathways of cadmium sulfide have been investigated. The results indicated that under ambient conditions, wz-CdS is the stable phase, while under high temperature and pressure conditions, rs-CdS becomes the stable phase. By investigating phase transformation pathways among wz-CdS, zb-CdS and rs-CdS, it has been found that zb-CdS is an intermediate phase in the transformation from rs-CdS to wz-CdS. Therefore, although there are no zb-CdS phase regions in the CdS pressure–temperature phase diagram, zb-CdS can be found in some prepared experiments.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (Grant No. 51121061, 51131002, and 51372215), the Key Basic Research Program of Hebei Province of China (Grant No. 12965135D) and the Natural Science Foundation for Distinguished Young Scholars of Hebei Province of China (Grant No. E2013203265). R.M. acknowledges the support from the NSERC and CRC programs, Canada. The authors also would like to thank the staff of the Center for Computational Materials Science, Institute for Materials Research, Tohoku University for computer support. Y.K. is thankful to the CREST project headed by Prof. M. Kotani.

References

1 P. Zhou, X. Q. Wang, M. Zhou, C. H. Xia, L. N. Shi and C. H. Hu, *Acta Phys. Sin.*, 2013, **62**, 087104.
2 C. X. Li and S. H. Dang, *Acta Phys. Sin.*, 2012, **61**, 17202.
3 G. Xin, J. Shen and D. Liu, *J. Dalian Univ. Technol.*, 2012, **52**, 157.
4 B. Wen and R. V. N. Melnik, *Appl. Phys. Lett.*, 2008, **92**, 261911.
5 J. J. Tan, Y. Li and G. F. Ji, *Acta Phys. Pol., A*, 2011, **120**, 501.
6 H. Cao, G. Wang, S. Zhang, X. Zhang and D. Rabinovich, *Inorg. Chem.*, 2006, **45**, 5103.
7 M. Knudson, Y. Gupta and A. Kunz, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1999, **59**, 11704.
8 O. Zakharov, A. Rubio, X. Blase, M. Cohen and S. Louie, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1994, **50**, 10780.
9 N. Stoffel, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1983, **28**, 3306.
10 T. Makino, K. Matsuishi, S. Onari and T. Arai, *J. Phys.: Condens. Matter*, 1998, **10**, 10919.

11 X. S. Zhao, J. Schroeder, T. Bilodeau and L. G. Hwa, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1989, **40**, 1257.

12 U. Venkateswaran and M. Chandrasekhar, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1985, **31**, 1219.

13 J. A. Corll, *J. Appl. Phys.*, 1964, **35**, 3032.

14 S. M. Antao and I. Hassan, *Can. Mineral.*, 2010, **48**, 1225.

15 K. Parlinski, *Journal of Physics: Conference Series*, 2007, IOP Publishing, p. 012009.

16 B. Wen, T. Shao, R. Melnik, Y. Kawazoe and Y. Tian, *J. Appl. Phys.*, 2013, **113**, 103501.

17 W. Yu, W. Lau, S. Chan, Z. Liu and Q. Zheng, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2003, **67**, 014108.

18 A. Siegel, K. Parlinski and U. Wdowik, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2006, **74**, 104116.

19 M. Sternik and K. Parlinski, *J. Phys. Chem. Solids*, 2006, **67**, 796.

20 G. Kresse and J. Furthmüller, *Comput. Mater. Sci.*, 1996, **6**, 15.

21 D. M. Ceperley, *Phys. Rev. Lett.*, 1980, **45**, 566.

22 T. Suzuki, T. Yagi, S. i. Akimoto, T. Kawamura, S. Toyoda and S. Endo, *J. Appl. Phys.*, 1983, **54**, 748.

23 *Numerical Data and Functional Relationships in Science and Technology*, ed. O. Madelung, M. Scnölz, H. Weiss and L. Börnstein, Springer-Verlag, Berlin, 1982.

24 K. Parlinski, Z. Li and Y. Kawazoe, *Phys. Rev. Lett.*, 1997, **78**, 4063.

25 F. D. Murnaghan, *Am. J. Math.*, 1937, **59**, 235.

26 N. Benkhettou, D. Rached, B. Soudini and M. Driz, *Phys. Status Solidi B*, 2004, **241**, 101.

27 K. Wright and J. D. Gale, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2004, **70**, 035211.

28 M. Kuball, J. Hayes, A. Prins, N. Van Uden, D. Dunstan, Y. Shi and J. Edgar, *Appl. Phys. Lett.*, 2001, **78**, 724.

29 S. Ouendadji, S. Ghemid, H. Meradji and F. Hassan, *Comput. Mater. Sci.*, 2011, **50**, 1460.

30 H. Iwanaga, A. Kunishige and S. Takeuchi, *J. Mater. Sci.*, 2000, **35**, 2451.

31 J. Sun, D. D. Klug and R. Martonak, *J. Chem. Phys.*, 2009, **130**, 194512.

32 C. Mailhiot and A. McMahan, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1991, **44**, 11578.

33 M. Catti, *Phys. Rev. Lett.*, 2001, **87**, 035504.

34 T. Hahn, U. Shmueli, A. A. J. C. Wilson and E. Prince, *International tables for crystallography*, D. Reidel Publishing Company, 2005.

35 M. Y. Lü, Z. W. Chen, L. X. Li, R. P. Liu and W. K. Wang, *Acta Phys. Sin.*, 2006, **55**, 3576.

36 P. Vajeeston, P. Ravindran and H. Fjellvåg, *J. Alloys Compd.*, 2007, **446**, 44.

37 V. Ozolins, E. Majzoub and C. Wolverton, *Phys. Rev. Lett.*, 2008, **100**, 135501.

38 Y.-S. Lee, Y. Kim, Y. W. Cho, D. Shapiro, C. Wolverton and V. Ozoliņš, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 2009, **79**, 104107.

39 H. L. Ni, Y. Liu, C. L. Song, G. Xu and G. R. Han, *Rare Met. Mater. Eng.*, 2008, **37**, 623.

40 J. P. Enríquez and X. Mathew, *Sol. Energy Mater. Sol. Cells*, 2003, **76**, 313.