Atomistic study of zinc-blende CdS, CdSe, ZnS, and ZnSe from molecular dynamics

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Abstract

Empirical interatomic potential parameters are determined for group semiconductors such as CdS, CdSe, ZnS, and ZnSe. The structural properties of zinc-blende CdS, CdSe, ZnS, and ZnSe are calculated. A good agreement between the calculated and experimental values of the lattice constant, the cohesion energy, and bulk modulus and its derivative are obtained. The versality of these empirical potential parameters is confirmed by the calculation of elastic constants for CdS, CdSe, ZnS, and ZnSe. We have used the molecular-dynamics methods for the calculations of the thermal expansion and heat capacity. The results compare well with available results. © 2000 Elsevier Science S.A. All rights reserved.

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1. Introduction

There are several theoretical models dealing with the subband structure of narrow-band-gap semiconductors. Technological and theoretical interest in II–VI compounds and their alloys in either wurtzite or zinc-blende structures has been growing recently due to its appealing properties in electro-optical and electron-acoustic devices [1–4]. ZnS, ZnSe, and ZnTe are the prototype II–VI semiconductors and their cubic phase, which occurs naturally as a mineral, has been called the zinc-blende structure. Considerable efforts is being devoted to realize a p-type material by doping or growing with impurities such as Li or Cl. When doped with Mn, the Zn-based W crystals form an interesting group of dilute magnetic semiconductors [5–7]. Futhermore, in recent years ZnSe has proved to be a particularly interesting dilute magnetic semiconductor when doped with Mn [8–10], many efforts have been made to fabricate a sustainable ZnSe blue laser. Finally, the very recent molecular-beam-epitaxy (MBE) growth of bcc Fe and Ni single crystals on ZnSe [11,12] is opening up the possibility of using such materials as microelectronic magnetic switches.

From the theoretical point of view, many authors have studied this semiconductor in order to explore, in more detail, its electronic properties, using various computers [13–15]. Some calculations [16] have ignored the Zn 3d orbitals, assuming them to part to the chemically inert atomic cores. Though a dramatic reduction in computer time has been achieved, the ignorance of the contribution of the Zn 3d electrons to chemical bonding in semiconductors may cause problems in depicting physical properties of the material. Photoemission spectra [17,18] show evidence of cation d bands and some recent calculations [19,20] treating the cation d electrons as valence electrons have indicated that the cation d electrons may play a significant role in II–VI and III–V semiconductors. However, the ground-state structural and cohesive properties of this material have not been widely investigated as it has been done for other semiconductors (e.g., GaAs or AlAs). The crystals SiC, ZnS, CdS, etc. exist in both forms: the structure Wurtzite (space group C_{6v}^4) form, which differs from the zinc-blende structure (group space T_d^2). Mainly at the relative positions of the third neighbors and beyond. The local atomic environments in both crystals are sufficiently close and it has been taken for granted that their electronic structures should also be very similar. In comparison with wurtzite structure very little is known about the electronic, optical and mechanical properties of zinc-blende II–VI under higher pressure and temperature. Moreover, the zinc-blende phase is hoped to be more amenable to doping than the wurtzite phase, since all of the semiconductor which can be efficiently doped are

cubic. Therefore, it is meaningful to characterize theoretically the physical properties of cubic (CdS, CdSe, ZnS, and ZnSe). In order to understand the nature of zinc-blende structure in high temperature it is necessary to use some form of microscopic modeling or simulation. The method used in the last reference is based on a dynamic molecular simulation method. The experience of the past two decades has shown that molecular dynamics calculations can provide a valuable tool to investigate nonharmonic effects in solids [21].

The advantages of the computational approach is that it can provide a much clearer atomic and electronic picture of the materials and their influences on the structures, properties, synthesis and performances. Empirical interatomic potentials for semiconductors have been proposed by many authors for application to dynamic treatments such as the molecular dynamics method for use in the simulation of complex systems with a large number of atoms, where the application of the first-principles methods us currently limited by the large computational effort. In attempting to explain the universal cohesive energy curves for various materials, we have use the empirical interatomic potentials of the Tersoff which include the three body interatomic interactions [22].

We predict with this approach, the behavior of solid CdS, CdSe, ZnS, and ZnSe under temperature and pressure effect. These potentials parameters are tested by calculating the elastic constants for II–V compounds semiconductors, equilibrium lattice parameters, bulk modulus, pressure derivatives, and cohesive energies in the cubic phase. We tested with this parameters the transferability of the potential by calculating the thermal expansion coefficient and the specific heat.

The paper is organized as follows. In Section 2 we give a brief description of the model used and calculation method. Then, the results of our calculation are presented and discussed in Section 3. Finally, a conclusion is given in Section 4.

2. Simulation details

The Tersoff potential is based in the bond-order concept [22,23]. The interatomic potential energy between two neighboring atoms i and j is written as

$$V_{ij} = f_c(r_{ij})[A \exp(-\lambda_1 r_{ij}) - B b_{ij} \exp(-\lambda_2 r_{ij})] \quad (1)$$

$$f_c(r_{ij}) = \begin{cases} 1, & r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left[\frac{\pi}{2}\frac{(r-R)}{D}\right], & R-D < r < R+D \\ 0, & r > R + D \end{cases} \quad (2)$$

where b_{ij} is the many-body bond-order parameter describing how the bond-formation energy (the attractive part of V_{ij}) is

affected by local atomic arrangement due to the presence of other neighboring atoms — the k atoms. It is a many-body function of the positions of atoms i, j and k. It has the form [22].

$$b_{ij} = (1 + \beta^n \xi_{ij}^{n_i})^{-1/(2n)} \quad (3)$$

with

$$\xi_{ij} = \sum_{k \neq i,j} f_c(r_{ij}) g(\theta_{ijk}) \exp[\lambda_3^3 (r_{ij} - r_{ik})^3] \quad (4)$$

$$g(\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta)^2} \quad (5)$$

$$a_{ij} = (1 + \alpha^n \eta_{ij}^n)^{-1/(2n)} \quad (6)$$

$$\eta_{ij} = \sum_{k \neq i,j} f_c(r_{ik}) \exp[\lambda_3^3 (r_{ij} - r_{ik})^3] \quad (7)$$

where ξ is called the effective coordination number and $g(\theta)$ a function of the angle between r_{ij} and r_{ik} that has been fitted to stabilize the tetrahedral structure. The potential parameters A, B, λ_1, λ_2, n, β, h, c and d are determined by heat of formation, cohesive energy, bulk modulus and the relative stability of various structures obtained from calculations and experiments [24–30]. We note that λ_3 and α are set equal to zero [31]. The parameters are fitted to polytype energies. Table 1 gives the adjusted parameters of (CdS, CdSe, ZnS, and ZnSe).

2.1. Computer simulations

Molecular dynamics (MD) is a direct simulation technique at the atomic level. Almost all the physical properties of a material may be determined using molecular dynamics. It requires generally an inter-particle potential. Thus, molecular-dynamic computer simulations have been performed to determine the prediction of Tersoff potential for solid structure under temperature and pressure effect. The MD cell is formed of a cube of side L with $3 \times 3 \times 3$ diamond units cells, where 216 particles are included. The periodic boundary conditions are applied. The atomic structure of solid has been calculated by using the canonical

Table 1
The adjusted Tersoff parameters for CdS, CdSe, ZnS, and ZnSe

	CdS	CdSe	ZnS	ZnSe
A (eV)	4129.0	5229.0	2475.8	3068.0
B (eV)	230.5	252.5	225.5	195.5
λ_1 (Å^{-1})	3.1299	3.1299	3.0099	3.1099
λ_2 (Å^{-1})	1.7322	1.7322	1.7322	1.7322
β	1.1×10^{-6}	1.5724×10^{-6}	1.1×10^{-6}	1.1×10^{-6}
n	0.78734	0.78734	0.78734	0.78734
c	100390	100390	100390	100390
d	16.217	16.217	16.217	16.217
h	−0.59825	−0.57058	−0.59825	−0.59825
R (Å)	3.059	3.175	3.059	2.99
D (Å)	0.15	0.15	0.15	0.15

NVT-ensemble. The MD routine is based on a fifth-order Gear–Predictor–Corrector algorithm of the Newtonian equations of motion using a neighbor list technique with a time step $\Delta t = 1.86$ fs, and an efficient network cube algorithm for nearest-neighbor book keeping, details are given elsewhere [32].

After an equilibration period, a histogram of atomic separations is produced in order to compute the pair distribution function [33] $g(r)$, and other various properties which are computed along the trajectory of the system in phase space.

2.2. Calculation of the elastic moduli

The elastic moduli of a cubic crystal may be divided into two classes, the bulk modulus $B=(C_{11}+2C_{12})/3$, and the two shear moduli $(C_{11}-C_{12})$, and C_{44}. The bulk modulus is related to the curvature of $E(V)$

$$B(V) = -VP'(V) = VE''(V) \tag{8}$$

where V is the volume of the unit cell, $E(V)$ the energy/unit cell at volume V, and $P(V)=-E'(V)$ is the pressure required to keep the cell at volume V. Begin by making a least-squares fit of the computed energies to the form proposed by Birch [34].

$$E(V) = E_0 + \frac{9}{8}B_0 V_0 \left[\left(\frac{V_0}{V}\right)^{2/3} - 1 \right]^2$$
$$+ \frac{9}{16}B_0(B_0'-4)V_0 \left[\left(\frac{V_0}{V}\right)^{2/3} - 1 \right]^3$$
$$+ \sum_{n=4}^{N} \gamma_n \left[\left(\frac{V_0}{V}\right)^{2/3} - 1 \right]^n \tag{9}$$

where E_0, B_0, and B_0' are, respectively, the equilibrium energy, volume, bulk modulus, and pressure derivative of the bulk modulus, while N is the order of the fit.

The shear moduli require knowledge of the derivative of the energy as a function of a lattice strain [35]. In the case of a cubic lattice, it is possible to choose this strain so that the volume of the unit cell is preserved. The strain can be chosen so that the energy is an even function of the strain, whence an expansion of the energy in powers of the strain contains no odd powers. Thus, for the calculation of the modulus $C_{11}-C_{12}$. We have used the volume-conserving orthorhombic strain tensor,

$$\vec{\varepsilon} = \begin{pmatrix} \delta & 0 & 0 \\ 0 & -\delta & 0 \\ 0 & 0 & \dfrac{\delta^2}{(1-\delta^2)} \end{pmatrix} \tag{10}$$

Application of this strain changes the total energy from its unstrained value to

$$E(\delta) = E(-\delta) = E(0) + (C_{11}-C_{12})V\delta^2 + O[\delta^4] \tag{11}$$

where V is the volume of the unit cell and $E(0)$ the energy of the unstrained lattice at volume V, and the strain parameter is defined as $\delta \equiv (\epsilon_\perp - \epsilon_{||})/3$ where $\epsilon_\perp$ is the strain along the [0 0 1] direction and $\epsilon_{||}$ the strain in the (0 0 1) plane.

Note that there is no pressure or stress term [36] in (11) since the strain (10) are constructed so that $\Delta V=0$.

The strain (10) can be used for any cubic lattice. In the general case, the internal parameters of the lattice must be chosen to minimize the total energy of the strained structure. Fortunately, the lattices discussed here fall into a restricted subset of the cubic lattices, where all of the atoms sit at inversion sites, even under the reduced symmetry caused by the strain (10).

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{12}$$

just as for a cubic crystal [38].

3. Results

3.1. Structural properties

3.1.1. Partial pair distribution function
In order to test the stability of our zinc-blende structure of CdS, CdSe, ZnS, and ZnSe at finite temperature within the Tersoff potential model, we have calculated the pair distribution functions, at 300 and 900 K. Fig. 1 shows the pair distribution function of CdS, CdSe, ZnS, and ZnSe. In Table 2, the amplitude and peaks positions are given.

The first peak position is 2.43, 2.61, 2.31, and 2.44 Å for CdS, CdSe, ZnS, and ZnSe, respectively, they represent the distance between a zinc-blende lattice point and its first neighboring tetrahedral site. The coordination numbers are evaluated by the equation

$$\eta = 4\pi\rho_0 \int r^2 \rho(r)\,\mathrm{d}r \tag{13}$$

where ρ_0 is the number density of atoms. The calculated and experimental [35] results are given in Table 2. Good agreement is observed.

3.1.2. Ground-state properties
Ground-state properties of CdS, CdSe, ZnS, and ZnSe were calculated within the Tersoff potential model by using MD simulation. The calculated ground-state energies plotted as functions of the volume for CdS, CdSe, ZnS, and ZnSe are shown in Fig. 2 in the zinc-blende phase. The equilibrium parameters from the Birch equation [34] fit (E_0, V_0, B_0, and B_0') are listed in Table 3. The calculated structural properties of CdS, CdSe, ZnS, and ZnSe are in good agreement with the room-temperature experimental and theoretical data. The equilibrium lattice constant is very close to the experimental value [24–26] with only a 0.05–0.07% deviation for CdS, CdSe, ZnS, and ZnSe, respectively.

Our values of bulk modulus are also in agreement with the experimental values [27,28]. The differences between
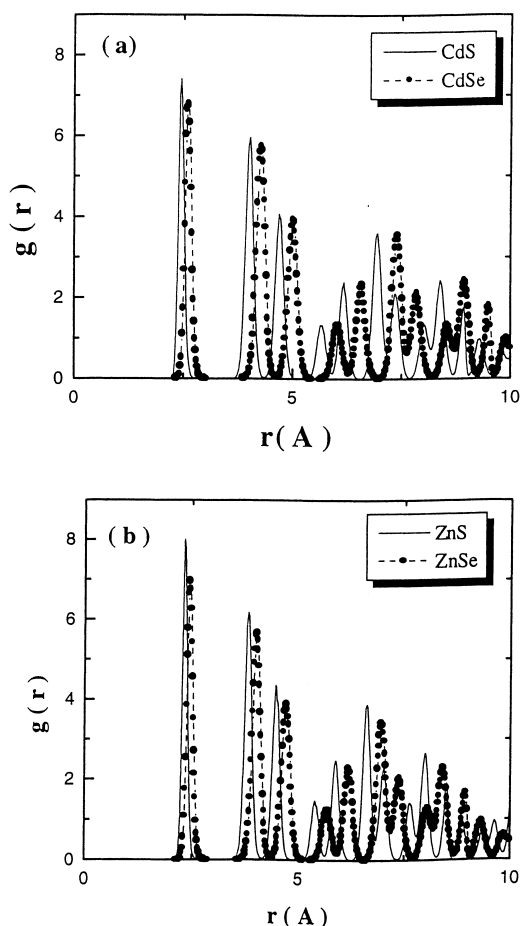
Fig. 1. Partial pair distribution functions for CdS, CdSe (a), ZnS, and ZnSe (b).

Fig. 2. Calculated total energies of CdS, ZnS (a), CdSe, and ZnSe (b) in the zinc-blende structure as a function of volume *V*.

calculated II–V modulus and experimental data [27,28] are within 3.2–9% for CdS, CdSe, ZnS, and ZnSe, and, respectively.

It is interesting to compare our results for B_0 with the values obtained using the empirical relation [39] $B_0 = (1971 - 220\lambda)d^{-3.5}$, where d is the nearest-neighbor distance in Angstroms. This relation is appropriate for the group-IV ($\lambda=0$), III–V ($\lambda=1$), and II–VI ($\lambda=2$) semiconductors. This relation gives $B_0=0.60$, 0.52, 0.78, and
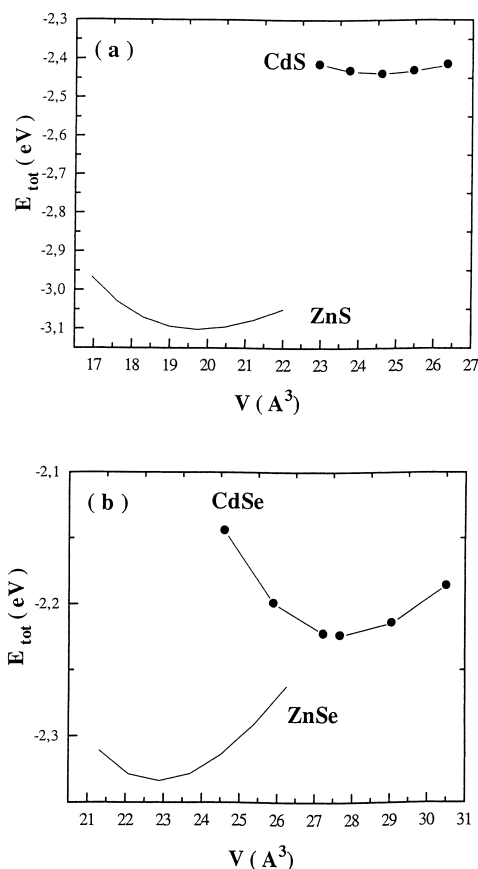
0.66 Mbar for CdS, CdSe, ZnS, and ZnSe, respectively, in excellent agreement with our results. The calculated results reported in Table 3 show that the Tersoff potential describes well the homogeneous response of group CdS, CdSe, ZnS, and ZnSe to hydrostatic compression.

3.1.3. Elastic properties

Knowledge of the elastic moduli of a given system is a first step in understanding its mechanical properties. In addition, the structural stability of a crystal when the system is under no external loading [37] is governed by elastic

Table 2

The values of peak distances and coordinate numbers of pairs for CdS, CdSe, ZnS, and ZnSe in the zinc-blende structure at 300 K[a]

	CdS	GdSe	ZnS	ZnSe
1st peak	Distance (Å): 2.434 (2.456)	2.615 (2.62)	2.319 (2.34)	2.442 (2.457)
	Number of pair: 3.97 (4)	3.97 (4)	3.970 (4)	4.009 (4)
2nd peak	Distance (Å): 4.01 (4.011)	4.267 (4.279)	3.811 (3.822)	4.014 (4.012)
	Number of pair: 11.927 (12)	11.935 (12)	11.936 (12)	12.099 (12)
3rd peak	Distance (Å): 4.681 (4.703)	5.012 (5.017)	4.46 (4.481)	4.714 (4.704)
	Number of pair: 11.966 (12)	11.942 (12)	11.997 (12)	12.084 (12)
4th peak	Distance (Å): 5.686 (5.674)	6.065 (6.053)	5.384 (5.406)	5.688 (5.675)
	Number of pair: 5.883 (6)	6.008 (6)	6.032 (6)	6.15 (6)

[a] Experimental values between brackets (from Ref. [35]).

Table 3
The calculated equilibrium lattice constant (Å), bulk moduli (Mbar), the pressure derivatives and the cohesive energies (eV) for CdS, CdSe, ZnS, and ZnSe in the zinc-blende structure at 300 K

System		CdS	CdSe	ZnS	ZnSe
a (Å)	Present work	5.815	6.055	5.406	5.667
	Calculated	5.819[a], 5.811[b]	6.05[a]	5.404[a], 5.345[b]	5.681[a], 5.618[b]
	Experimental	5.818[c]	–	5.410[d]	5.667[e]
B (Mbar)	Present work	0.623	0.546	0.816	0.590
	Calculated	0.60[a]	0.52[a]	0.78[a]	0.66[a]
	Experimental	0.644[f]	–	0.78[g]	0.595[g]
B'	Present work	5.466	5.57	4.73	5.41
E_{coh} (eV)	Present work	−2.437	−2.224	−3.102	−2.287
	Calculated	–	–	–	–
	Experimental	–	–	3.165[h]	2.19[h]

[a] Ref. [39].
[b] Ref. [40].
[c] Ref. [24].
[d] Ref. [25].
[e] Ref. [26].
[f] Ref. [27].
[g] Ref. [28].
[h] Ref. [29,30].

constants. The comparison of the calculated moduli provides a meaningful test of the interatomic potential function. We have determined the elastic constants at 300 K: C_{11} and C_{12} from Eq. (11) combined with Eq. (12).
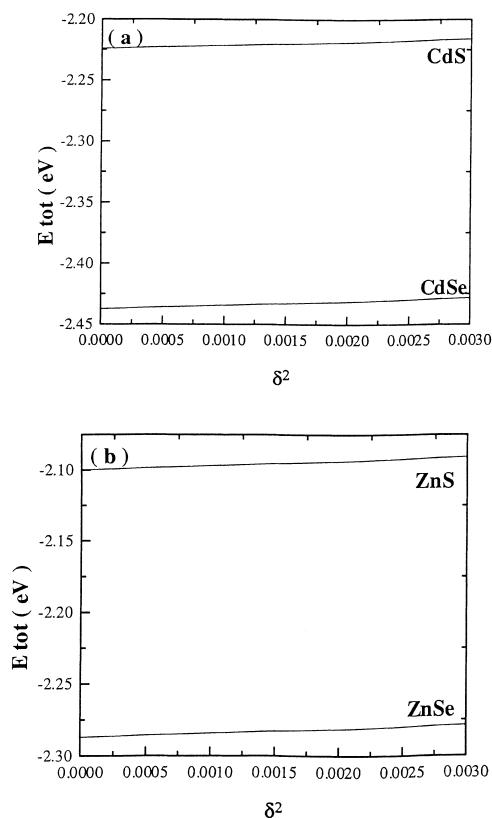

Fig. 3 displays the energy of CdS, CdSe, ZnS, and ZnSe as a function of orthorhombic strain (10) for the fixed volume associated with the cubic lattice constant $a_{CdS}=5.815$, $a_{CdSe}=6.055$, $a_{ZnS}=5.406$, and $a_{ZnSe}=5.667$ Å The slope of the these curves yield $C_{11}-C_{12}$ according to Eq. (11). Table 4 gives the elastic constants C_{11} and C_{12}, with some data of literature [28]. A good agreement is observed for the elastic constant.

3.2. Thermal properties

The thermal expansion coefficient α measures how the lattice constant responds to an isometric change in temperature,

$$\alpha = \frac{1}{a}\left(\frac{\partial a}{\partial T}\right)_P \qquad (14)$$

The thermal expansion coefficient at room-temperature is then computed from the temperature derivative of these lattice constants. At temperatures below the Debye tempera-

Table 4
Equilibrium constants for cubic structure[a]

System		CdS	CdSe	ZnS	ZnSe
C_{11}	Simulated	0.752	0.650	0.980	0.72
	Calculated	–	–	–	–
	Experimental	–	–	1.04[b]	0.81[b]
C_{12}	Simulated	0.55	0.49	0.73	0.52
	Calculated	–	–	–	–
	Experimental	–	–	0.65[b]	0.488[b]

[a] Compared with theoretical and experimental calculation at $T=300$ K for CdS, CdSe, ZnS, and ZnSe in the zinc-blende structure.
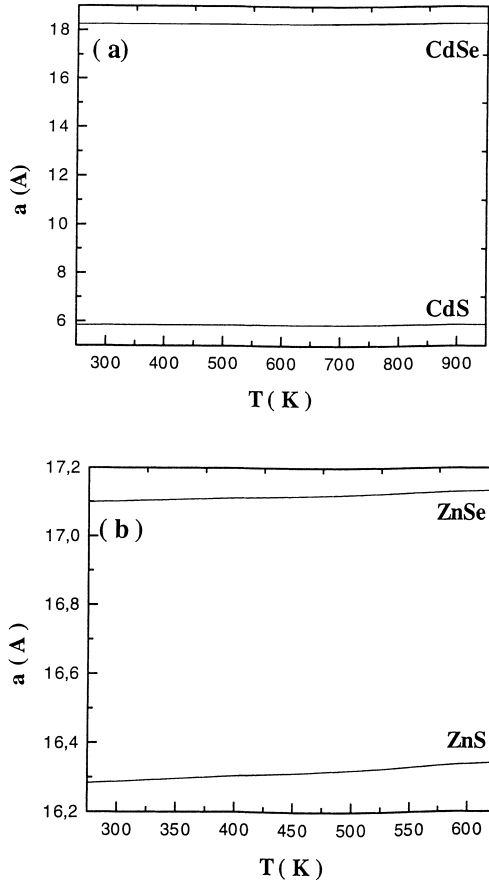[b] Ref. [28].

Fig. 3. Energy as a function of the square of the orthorhombic strain (10) for CdS, CdSe (a), ZnS, and ZnSe (b).

Fig. 4. The lattice constant of system for CdS, CdSe (a), ZnS, and ZnSe (b) as function of temperature.

Fig. 5. The total energy of the system as function of temperature for CdS, CdSe (a), ZnS, and ZnSe (b).

ture, quantum effects are important in determining thermal expansion. Above the Debye temperature, quantum effects become unimportant, and thermal expansion may be determined from classical calculations, such as molecular dynamics (MD). Thermal expansion is due to anharmonic terms in the cohesive energy for small displacements of the atom about its equilibrium position at 0 K. The thermal expansion of CdS, CdSe, ZnS, and ZnSe has been studied in the temperature range from 300 to 900 K.

Fig. 4 shows the variations of the lattice parameter of CdS, CdSe, ZnS, and ZnSe with temperature. The collected data can be fitted to polynomial functions of temperature as:

$$a_{CdS} = 5.83 + 4 \times 10^{-5} T \tag{15}$$

$$a_{CdSe} = 6.089 + 2 \times 10^{-5} T \tag{16}$$

$$a_{ZnS} = 5.412 + 6 \times 10^{-5} T \tag{17}$$

$$a_{ZnSe} = 5.690 + 3 \times 10^{-5} T \tag{18}$$

The linear temperature coefficients determined from Eq. (15) to Eq. (18) are $(0.68, 0.33, 1.10, 0.529) \, 10^{-5} \, K^{-1}$ of CdS, CdSe, ZnS, and ZnSe, respectively. The results are in good order of many other semiconductors with zinc-blende structure, indicating that the average anharmonicity of the interactions in the Tersoff potential is reasonable.
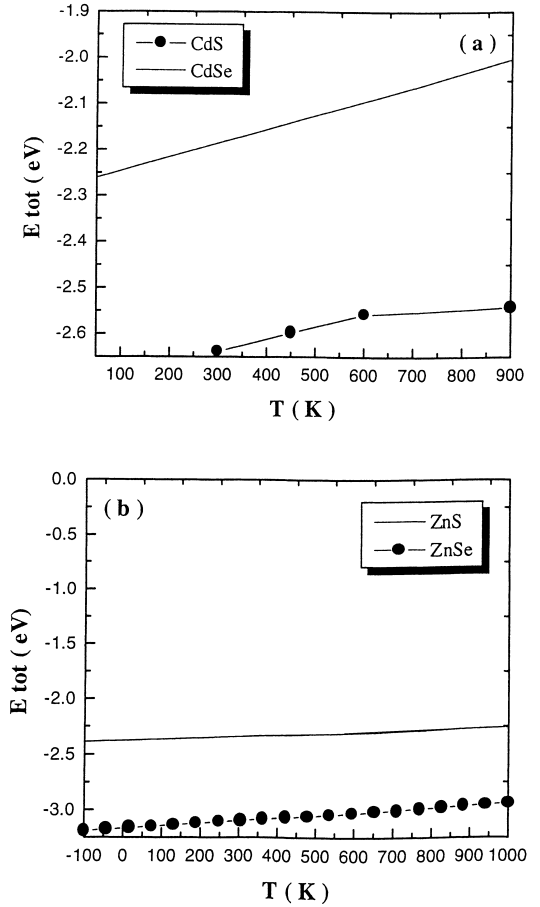
The specific heat of CdS, CdSe, ZnS, and ZnSe at constant volume (C_v) is also calculated using the Tersoff potential. The constant-volume heat capacity measures how the internal energy responds to an isometric change in temperature,

$$C_v = \left(\frac{\partial E}{\partial T} \right)_V \tag{19}$$

From Fig. 5 we determine the specific heat of CdS, CdSe, ZnS, and ZnSe, C_v=6.01, 5.58, 5.29, and 6.211 cal K^{-1} mol^{-1}, respectively. This result is certainly in agreement with experiment at high temperature, where the value of specific heat is close to $3R$, where R is the universal gas constant ($R \approx 2$ cal K^{-1} mol^{-1}) for CdS, CdSe, ZnS, and ZnSe. This range usually includes room temperature. The fact that is nearly equal to $3R$ at high temperatures regardless of the substance described is called the Dulong–Petit law.

4. Conclusion

We have proposed empirical potentials of Tersoff parameters for CdS, CdSe, ZnS, and ZnSe. We have tested the validity of our fitting of empirical interatomic potentials

parameters by calculating the structural and elastics properties for CdS, CdSe, ZnS, and ZnSe compounds semi-conductors. The results exhibit excellent agreement with available experimental data. The result of the thermal expansion and specific heat of CdS, CdSe, ZnS, and ZnSe are in the same order of many other semiconductors with zinc-blende structure.

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