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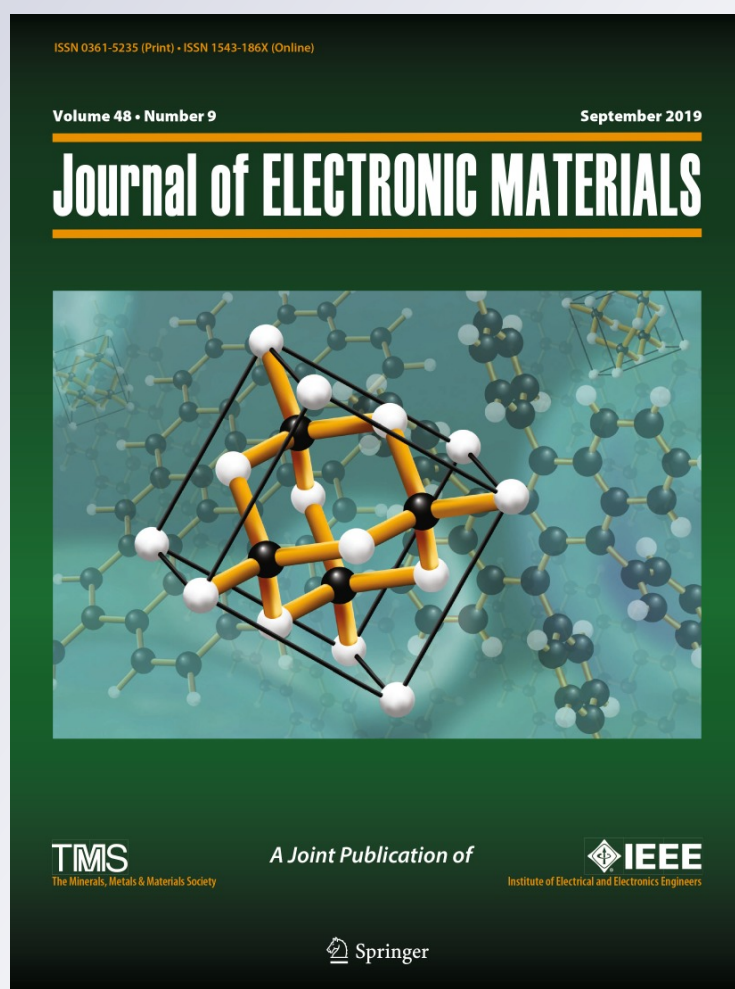
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Structural and Thermomechanical Properties of Zincblende-Type ZnX (X = S, Se, Te)

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The structural and thermomechanical properties of zincblende ZnX (X = S, Se, Te) compounds have been investigated based on the moment method in statistical mechanics. Expressions for the lattice constant, atomic mean-square displacement (MSD), and elastic moduli (Young's modulus, bulk modulus, and shear modulus) of the zincblende compounds were derived. The results show that the quantum-mechanical zero-point vibrations make the main contribution to the atomic MSDs at low temperature. At high temperature, due to the predominance of anharmonicity, the atomic MSDs increase rapidly with increasing temperature. The Young's modulus and shear modulus of the zinc chalcogenides ZnX (X = S, Se, Te) were calculated. The data derived from this research can be seen as useful references for future experiments.

Key words: Thermodynamic properties, mean-square displacement, mechanical properties, elastic modulus, ZnX

INTRODUCTION

The zinc chalcogenides ZnX (X = S, Se, Te) are of great interest not only from a fundamental point of view but also for technological and electronic applications. These materials are known for their wide band gap, which makes them potential candidates for many high-technology applications such as photovoltaic devices,¹ photodetectors,² blue light-emitting diodes,³ solar cells,⁴ and catalyst applications. Hence, great effort has been devoted to obtaining deeper understanding of the physical properties of these compounds. Besides their many interesting properties, zinc chalcogenides show several structural phases at various

temperatures and pressures. The two main phases at ambient conditions have zincblende and wurtzite structure.⁵ Although extensive experimental and theoretical studies on ZnX (X = S, Se, Te) compounds have been reported, investigation of their thermomechanical properties remains very limited.⁶ Most previous studies on ZnX (X = S, Se, Te) focused on the lattice parameter, bulk modulus, and elastic constants.^{7–9} To the best of the authors' knowledge, almost no measurements have been performed on the Young's modulus or shear modulus of zincblende-type zinc chalcogenides ZnX (X = S, Se, Te). Furthermore, while anharmonic effects make important contributions to thermodynamic quantities at high temperature, most previous theoretical works have found it difficult to take into account the anharmonicity of thermal lattice vibrations, especially above the Debye temperature.

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In the work presented herein, a statistical-mechanical method, viz. the so-called statistical moment method (SMM), is applied to compounds with zincblende structure. We investigate the structural and thermomechanical properties of ZnX (X = S, Se, Te), considering the anharmonicity of the thermal lattice vibrations. Expressions for the temperature-induced atomic displacements, nearest-neighbor distances between two intermediate atoms, atomic mean-square displacements, Young's modulus, bulk modulus, and shear modulus of zincblende ZnX (X = S, Se, Te) compounds are derived based on the moment expansion technique in the SMM scheme.

The remainder of this manuscript is organized as follows: In "Theory" section, the theoretical approach to the investigation of the thermomechanical properties of zincblende compounds is presented, then numerical calculations are performed for ZnX (X = S, Se, Te) in "Results and Discussion" section, where the numerical results are also discussed in detail. Finally, "Conclusions" section presents the conclusions of the current work.

THEORY

Thermal Lattice Vibrations

Firstly, we present fundamental results derived for materials with zincblende structure within the SMM scheme. Denote the interatomic potential as $\varphi(r)$. The SMM approach starts with consideration of the total force acting on a chosen central atom in the lattice. Due to thermal lattice vibrations, the 0th central atom is affected by a supplementary force p , such that the total force acting on it must be zero, thus the following force balance equation should be satisfied:

$$\begin{aligned} & \frac{1}{2} \sum_{\alpha, \delta} \left(\frac{\partial^2 \varphi_{i0}}{\partial u_{i\alpha} \partial u_{i\delta}} \right)_{eq} \langle u_{i\alpha} \rangle_p + \frac{1}{6} \sum_{\alpha, \delta, \gamma} \left(\frac{\partial^3 \varphi_{i0}}{\partial u_{i\alpha} \partial u_{i\delta} \partial u_{i\gamma}} \right)_{eq} \langle u_{i\alpha} u_{i\gamma} \rangle_p \\ & + \frac{1}{24} \sum_{i, \alpha, \gamma, \eta} \left(\frac{\partial^4 \varphi_{i0}}{\partial u_{i\alpha} \partial u_{i\delta} \partial u_{i\gamma} \partial u_{i\eta}} \right)_{eq} \langle u_{i\alpha} u_{i\gamma} u_{i\eta} \rangle_p - p = 0, \end{aligned} \quad (1)$$

where u_i is the displacement of the i th atom from its equilibrium position, φ_{i0} indicates the effective interaction energy between the 0th and i th atoms, and $\langle u_{i\alpha} u_{i\gamma} \rangle_p$ and $\langle u_{i\alpha} u_{i\gamma} u_{i\eta} \rangle_p$ are, respectively, the second- and third-order moments of the thermal average of the atomic displacement; the subscript "eq" denotes the thermal average taken over the equilibrium ensemble

Based on a recurrence formula in the SMM method,¹⁰ the power moments $\langle u_{i\alpha} u_{i\gamma} \rangle_p$ and $\langle u_{i\alpha} u_{i\gamma} u_{i\eta} \rangle_p$ can be expressed in terms of the first-order moment $\langle u_{i\alpha} \rangle_p$, and the differential Eq. 1 can be rewritten in the form

$$\begin{aligned} & \gamma \theta^2 \frac{d^2 y}{dp^2} + 3\gamma \theta y \frac{dy}{dp} + ky + \gamma \frac{\theta}{k} (X - 1)y + \beta \gamma \frac{dy}{dp} \\ & + \beta y^2 - p = 0, \end{aligned} \quad (2)$$

where

$$\begin{aligned} & y = \langle u_{i\alpha} \rangle = \langle u_{i\gamma} \rangle = \langle u_{i\eta} \rangle \equiv \langle u_i \rangle_p, \\ & X = \frac{\hbar \omega}{2\theta} \coth \left(\frac{\hbar \omega}{2\theta} \right), \quad \theta = k_B T, \end{aligned} \quad (3)$$

$$k = \frac{1}{2} \sum_i \left(\frac{\partial^2 \varphi_{i0}}{\partial u_{i\alpha}^2} \right)_{eq} = m \omega^2; \quad \beta = \left(\frac{\partial^3 \varphi_{i0}}{\partial u_{i\alpha} \partial u_{i\beta} \partial u_{i\gamma}} \right)_{eq}, \quad (4)$$

$$\gamma = \frac{1}{24} \sum_i \left[\left(\frac{\partial^4 \varphi_{i0}}{\partial u_{i\alpha}^4} \right)_{eq} + 6 \left(\frac{\partial^4 \varphi_{i0}}{\partial u_{i\alpha}^2 \partial u_{i\beta}^2} \right)_{eq} \right], \quad (5)$$

with $\alpha \neq \gamma \neq \eta = x, y$ or z directions in the Cartesian coordinate system, k_B the Boltzmann constant, and T the absolute temperature.

The solution of the nonlinear differential equation Eq. 2 can be written in the form

$$y'_0 = y_0 + A_1 p + A_2 p^2, \quad (6)$$

where A_1 and A_2 are constant coefficients,¹¹ and y_0 represents the atomic displacement taking into account the anharmonic effects of the thermal lattice vibrations of the zincblende-type semiconductor. The solution for the atomic displacement y_0 can be derived as¹¹

$$\begin{aligned} & y_0(T) = \sqrt{\frac{2\gamma \theta^2}{3K^3} A - \frac{\beta}{3\gamma} + \frac{1}{K} \left(1 + \frac{6\gamma^2 \theta^2}{K^4} \right)} \\ & \times \left[\frac{1}{3} - \frac{2\gamma \theta}{3k^2} (X - 1) - \frac{2\beta^2}{27\gamma k} \right] \frac{\beta k}{\gamma}, \end{aligned} \quad (7)$$

where $K = k - \beta^2/3\gamma$ and

$$A = a_1 + \frac{\gamma^2 \theta^2}{K^4} a_2 + \frac{\gamma^3 \theta^3}{K^6} a_3 + \frac{\gamma^4 \theta^4}{K^8} a_4 + \frac{\gamma^5 \theta^5}{K^{10}} a_5 + \frac{\gamma^6 \theta^6}{K^{12}} a_6, \quad (8)$$

where the quantities $a_1, a_2, a_3, a_4, a_5,$ and a_6 are defined as in Ref. 12.

The nearest-neighbor distance between two intermediate atoms at temperature T can now be determined as

$$r_1(T) = r_1(0) + y_0(T), \quad (9)$$

where $r_1(0)$ denotes the value of the nearest-neighbor distance at zero temperature, which can be calculated from the minimum condition of the

potential energy of the crystal. After deriving the nearest-neighbor distance, we evaluate the lattice constant $a_h(T)$ of the zincblende compound as $a_h(T) = \frac{4}{\sqrt{3}}r_1(T)$.

Atomic Mean-Square Displacement

The temperature-dependent atomic mean-square displacement or Debye–Waller factor $\langle u^2 \rangle$ is a thermodynamic quantity which measures the deviation of the thermal vibration of the atom. Theoretically, the mean-square displacement can be derived by using various approaches (lattice dynamic models,¹³ phonon density of states method¹⁴ or shell models,¹⁵ and density functional theory).¹⁶ Experimentally, the Debye–Waller factor $\langle u^2 \rangle$ can be measured by x-ray diffraction analysis,¹⁷ Mössbauer absorption,¹⁸ and neutron diffraction.¹⁹ To derive the mean-square displacement expression in the SMM scheme, we use the following relation between the first- and second-order moments.²⁰

$$\begin{aligned} \langle u_{ix}u_{i\gamma} \rangle_a &= \langle u_{ix} \rangle_a \langle u_{i\gamma} \rangle_a + \theta \frac{\partial \langle u_{ix} \rangle_a}{\partial a_\gamma} \\ &+ \frac{\hbar \delta_{x\gamma}}{2m\omega} \coth\left(\frac{\hbar\omega}{2\theta}\right) - \frac{\theta \delta_{x\gamma}}{m\omega^2}. \end{aligned} \quad (10)$$

Using this formula, an expression for the atomic mean-square displacement can be derived as

$$\langle u_i^2 \rangle = \langle u_i \rangle^2 + \theta A_1 + \frac{\theta}{k}(X - 1), \quad (11)$$

where

$$A_1 = \frac{1}{K} \left[1 + \frac{2\gamma^2\theta^2}{K^4} \left(1 + \frac{X}{2} \right) (X + 1) \right]. \quad (12)$$

In the low-temperature limit ($T \rightarrow 0$ K), the zero-point contribution to the mean-square displacement characterizing the quantum effect is obtained as

$$\langle u_i^2 \rangle_{T \rightarrow 0 \text{ K}} = \frac{\hbar\omega}{2k}. \quad (13)$$

In the high-temperature limit, the parameter $X = \frac{\hbar\omega}{2\theta} \coth\left(\frac{\hbar\omega}{2\theta}\right)$ will tend to 1, and the mean-square displacement function reduces to the simple form

$$\langle u_i^2 \rangle = \frac{\theta}{K} + \frac{6\gamma^2\theta^3}{K^5} + \frac{2\gamma\theta^2}{3K^3}A. \quad (14)$$

Elastic Moduli

The elastic moduli (characterized by the Young's modulus E , bulk modulus B , and shear modulus G) are important mechanical properties which affect the dynamic properties of a material.²¹ In previous work considering only lattice deformations due to an

external force, Hung and Hai²² derived the following analytical expression for the Young's modulus E in the SMM scheme based on the theory of lattice vibrations:

$$E \approx \frac{1}{\pi r_1 A_1} = \frac{1}{\pi [r_1(0) + y_0] A_1}, \quad (15)$$

where y_0 and A_1 have the same forms as in Eqs. 7 and 12, respectively.

The two other elastic moduli (bulk modulus B and shear modulus G) of the material can be derived based on the Young's modulus and Poisson's ratio as

$$B \approx \frac{E}{3(1 - 2\nu)}, \quad (16)$$

$$G = \frac{E}{2(1 + \nu)}, \quad (17)$$

where ν denotes the Poisson's ratio characterizing the stability of the crystal under shear deformation, being one of the essential parameters among the mechanical properties of a solid.

RESULTS AND DISCUSSION

The expressions derived in the previous section are now used to determine the lattice constants, temperature-dependent atomic mean-square displacements, and elastic moduli of the zincblende-type ZnX ($X = \text{S, Se, Te}$) compounds. To perform these numerical calculations, the interaction potential among atoms is assumed to be the many-body Stillinger–Weber potential,²³ which has usually been applied to study the physical properties of zincblende-type semiconductors.^{7,24–26} This type of many-body potential function, suggested by Stillinger and Weber,²³ consists of two-body (Φ_{ij}) and three-body (W_{ijk}) terms as follows:

$$\phi_i = \sum_j \Phi_{ij}(r_i, r_j) + \sum_{j,k} W_{ijk}(r_i, r_j, r_k), \quad (18)$$

with

$$\Phi_{ij}(r_i, r_j) = \begin{cases} A \left[B \left(\frac{r_{ij}}{\sigma} \right)^{-4} - 1 \right] \exp \left[\left(\frac{r_{ij}}{\sigma} - b \right)^{-1} \right], & \frac{r_{ij}}{\sigma} < b \\ 0, & \frac{r_{ij}}{\sigma} \geq b \end{cases} \quad (19)$$

and the three-body term corresponding to the angle distortion energy

$$\begin{aligned} W_{ijk}(r_i, r_j, r_k) &= \lambda \exp \left[\tau \left(\frac{r_{ij}}{\sigma} - b \right)^{-1} + \tau \left(\frac{r_{ik}}{\sigma} - b \right)^{-1} \right] \\ &\times \left(\cos \theta_{ijk} + \frac{1}{3} \right)^2, \end{aligned} \quad (20)$$

Table I. Stillinger–Weber potential parameters^{7,25} and Poisson's ratio²⁷ ν of zincblende ZnX (X = S, Se, Te) compounds

Compound	A (eV)	B	σ (Å)	τ	λ	b	ν
ZnS	7.6488	1.1496	2.3240	1.8367	32.50	2.0353	0.370
ZnSe	7.6841	0.6022	2.1864	1.2	31.61	1.80	0.399
ZnTe	9.9589	0.9852	2.1864	1.2	37.41	1.80	0.356

where the potential parameters A and B are positive, σ has dimensions of length, r_{ij} is the bond length between the i th and j th atom, θ_{ijk} is the angle between bonds ij and ik , and b is a dimensionless parameter representing the cutoff distance of the interaction. The potential parameters for ZnX (X = S, Se, Te) compounds are presented in Table I.^{7,25}

Tables II, III, and IV present the results of the calculations for the lattice constants and elastic moduli (Young's modulus, bulk modulus, and shear modulus) of the zincblende ZnX (X = S, Se, Te) semiconductors at room temperature. Previous experimental measurements^{8,28,29} and theoretical calculations [force field potential calculations,⁷ self-consistent tight-binding linear muffin-tin orbital (TB-LMTO) method,⁸ and pseudopotential plane wave (PP-PW) calculations³⁰] are also presented for comparison. As observed from these tables, the theoretical calculations presented herein are in agreement with previous results. The maximum difference between the results of this work and experiments is about 10%. Consequently, the derived values of the lattice constants can be used for further investigation. Figure 1 shows the calculated Young's modulus of ZnX (X = S, Se, Te) as a function of temperature. As observed from this figure, the Young's modulus E is a decreasing function of temperature, and the Young's modulus of ZnSe depends more strongly on temperature than those of ZnS and ZnTe. This indicates that the mechanical properties of ZnSe will change quickly from hard to soft as the temperature is increased. According to these calculations, the mean slope of the Young's modulus $|\Delta E/\Delta T|$ for the compounds ZnS, ZnSe, and ZnTe is 0.019 GPa/K, 0.035 GPa/K, and 0.017 GPa/K, respectively. Note that it seems that no experimental measurements have been performed to determine the Young's modulus or shear modulus of zincblende ZnX (X = S, Se, Te) compounds, thus we compare the results of our SMM calculations with values obtained from elastic constants.²⁷ Indeed, the predictions for the elastic moduli (Young's modulus, bulk modulus, and shear modulus) of zincblende ZnX (X = S, Se, Te) presented herein can be seen as useful references for future experiments. We hope that the theoretical findings of these thermomechanical quantities will be verified experimentally in the near future.

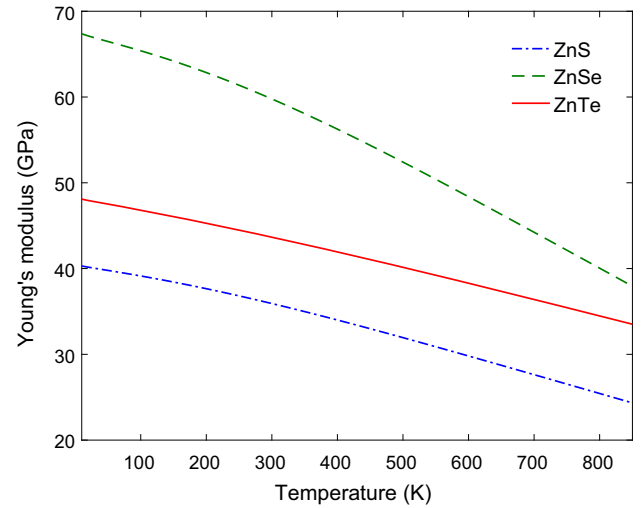


Fig. 1. (Color online) Temperature-dependent Young's modulus of ZnX (X = S, Se, Te).

While the elastic behavior of a material can be described by its elastic moduli (Young's modulus E , bulk modulus B , and shear modulus G), knowledge of the elastic constants provides important information concerning the stiffness, mechanical stability, and structural phase changes of the material.²¹ Due to the symmetry of the stress and strain tensors, the most general elastic stiffness tensor only has 21 nonzero independent components. For a cubic structure, this reduces to three independent elastic stiffness components, viz. C_{11} , C_{12} , and C_{44} . For an isotropic material, the elastic constants C_{11} , C_{12} , and C_{44} can be written in terms of the Young's modulus E and Poisson's ratio ν as follows:²²

$$C_{11} = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)}, \quad (21)$$

$$C_{12} = \frac{E\nu}{(1 + \nu)(1 - 2\nu)}, \quad (22)$$

$$C_{44} = \frac{E}{2(1 + \nu)}. \quad (23)$$

Using these formulae, the elastic constants C_{11} , C_{12} , and C_{44} of zincblende ZnX (X = S, Se, Te) can be easily derived and are also presented in

Table II. Lattice constant a_h , Young's modulus E , bulk modulus B , shear modulus G , and elastic constants of ZnS at temperature $T = 300$ K

	a_h (Å)	E (GPa)	B (GPa)	G (GPa)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Present method	5.4630	59.77	76.63	21.81	10.57	6.21	4.36
Experiments	5.4100 ^a	–	76.9 ^b	–	10.40, ^c 10.2 ^g	6.50, ^c 6.46 ^g	4.00, ^c 4.46 ^g
Calculations	5.3998, ^e 5.328 ^h 5.336 ⁱ	51.3 ^g	80.97, ^e 83.1 ^f 83.8, ^h 81.2 ⁱ	18.7 ^g	9.94, ^d 11.58 ^h	7.44, ^d 7.20 ^h	2.45, ^d 5.15 ^h

^aRef. 8.^bRef. 31.^cRef. 7.^dForce field potential calculations⁷.^eTB-LMTO method⁸.^fPP-PW calculations in Ref. 30.^gRef. 27.^hFirst-principles calculations in Ref. 32.ⁱFirst-principles calculations in Ref. 9.**Table III. Lattice constant a_h , Young's modulus E , bulk modulus B , shear modulus G , and elastic constants of ZnSe at temperature $T = 300$ K**

	a_h (Å)	E (GPa)	B (GPa)	G (GPa)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Present method	5.760	35.92	59.27	12.84	7.64	5.07	2.57
Experiments	5.667 ^a	–	69.3 ^b	–	8.57, ^b 8.10 ^c	5.07, ^b 4.90 ^c	4.05, ^b 4.40 ^c
Calculations	5.666, ^e 5.582 ^h	47.8 ^g	67.32, ^e 68.9 ^f 70.8 ^h	17.5 ^g	7.76 ^d	5.10 ^d	2.33 ^d

^ax-Ray diffraction measurements in Ref. 29.^bRef. 31.^cRef. 7.^dForce field potential calculations⁷.^eTB-LMTO method⁸.^fPP-PW calculations in Ref. 33.^gRef. 27.^hFirst-principles calculations in Ref. 9.**Table IV. Lattice constant a_h , Young's modulus E , bulk modulus B , shear modulus G , and elastic constants of ZnTe at temperature $T = 300$ K**

	a_h (Å)	E (GPa)	B (GPa)	G (GPa)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Present method	6.135	43.67	50.54	16.10	7.208	3.98	3.22
Experiments	6.009, ^a 6.089 ^b	–	52.8 ^b	–	7.10, ^c 7.15 ^f	4.10, ^c 4.08 ^f	3.10, ^c 3.11 ^f
Calculations	6.063 ^e	63.2 ^g	50.54 ^e	15.4 ^g	6.39 ^d	3.92 ^d	1.96 ^d

^aRef. 28.^bRef. 8.^cRef. 7.^dForce field potential calculations⁷.^eTB-LMTO method⁸.^fRef. 31.^gRef. 27.

Tables II, III, and IV. Our SMM results are in reasonable agreement with previous experimental measurements.^{7,27} The values in these tables also

demonstrate that the present SMM calculations of the elastic constants give slightly better results compared with force field potential calculations.⁷

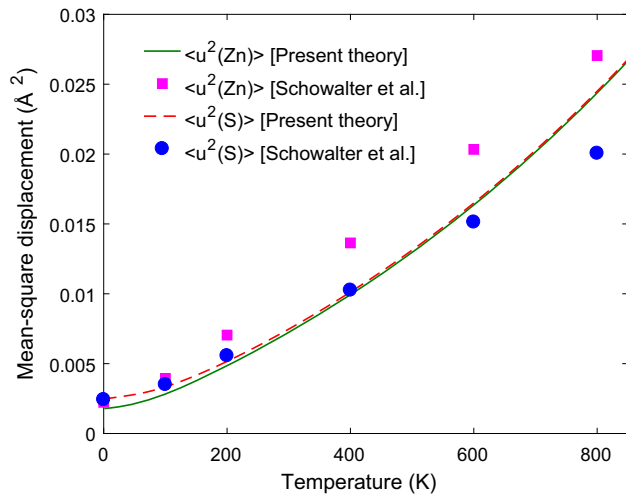


Fig. 2. (Color online) Temperature-dependent mean-square displacements of Zn and S. Density functional theory calculations performed by Schowalter et al.¹⁶ are shown for comparison.

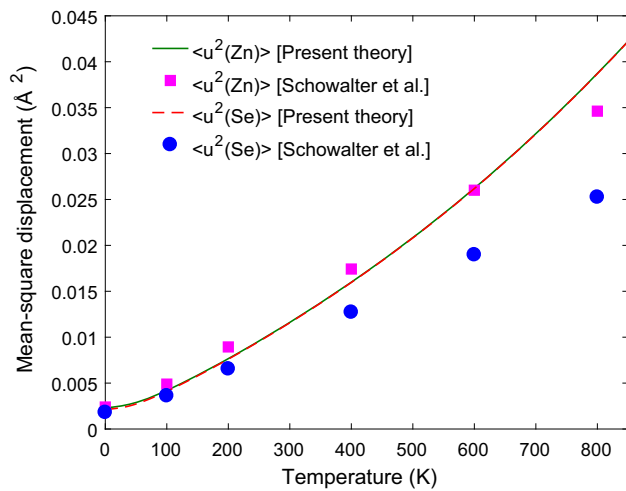


Fig. 3. (Color online) Temperature-dependent mean-square displacements of Zn and Se. Density functional theory calculations performed by Schowalter et al.¹⁶ are shown for comparison.

Figures 2, 3, and 4 present SMM calculations for the temperature-dependent mean-square displacements $\langle u^2 \rangle$ of atoms in the zincblende-type ZnX ($X = S, Se, Te$) compounds together with experimental measurements³⁴ and other theoretical results.^{15,16} As can be seen from these figures, the SMM results are in agreement with those of previous works^{15,16,34} at temperatures below 600 K. Beyond 600 K, a slight difference starts to appear. At low temperature $T \leq 50$ K, a quantum effect (zero-point vibration) can be observed from the mean-square displacement curves and the atomic vibration contribution of the light atom is greater than that of the heavier one in ZnX ($X = S, Se, Te$). In detail, the zero-point contributions of Zn and S in

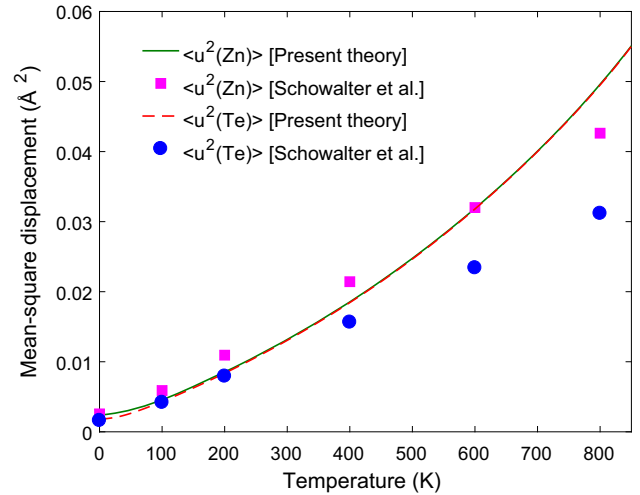


Fig. 4. (Color online) Temperature-dependent mean-square displacements of Zn and Te. Density functional theory calculations performed by Schowalter et al.¹⁶ are shown for comparison.

ZnS are, respectively, 0.0018 \AA^2 and 0.0025 \AA^2 ; those of Zn and Se in ZnSe are, respectively, 0.0021 \AA^2 and 0.0020 \AA^2 ; those of Zn and Te in ZnTe are, respectively, 0.0024 \AA^2 and 0.0018 \AA^2 . Table V presents the atomic mean-square displacements of Zn and X ($X = S, Se, Te$) atoms for the ZnX materials at room temperature. Interestingly, the ratio between the Debye-Waller factors of Zn and X ($X = S, Se, Te$) at zero temperature is almost equal to the square root of their inverse mass ratio, viz. $\sqrt{m(X)}/\sqrt{m(Zn)} \approx 0.7002, 1.0990, \text{ and } 1.3970$ for $X = S, Se, \text{ and } Te$, respectively. However, this difference between the mean-square displacements of Zn and X ($X = S, Se, Te$) progressively disappears as the temperature increases.

Furthermore, it is worth mentioning that the quantum-mechanical zero-point vibrations make the main contributions to the atomic mean-square displacements at low temperature. At high temperature, due to the predominance of anharmonicity due to the increasing oscillation amplitude of the atoms, the atomic mean-square displacements increase rapidly with increasing temperature. Equation 14 indicates that the temperature dependence of the mean-square displacement $\langle u^2 \rangle$ is specified by the factor θ^3 . This means that the atomic mean-square displacement function $\langle u^2 \rangle$ grows with temperature T to the power of 3.

CONCLUSIONS

The thermomechanical properties of ZnX ($X = S, Se, Te$) were investigated using the many-body Stillinger–Weber potential in the statistical-mechanical moment method formalism, providing analytical expressions for the lattice constant, atomic mean-square displacements, and elastic (Young's, bulk, and shear) moduli of zincblende-type semiconductors. The agreement between the present calculations

Table V. Comparison of atomic mean-square displacements (\AA^2) in zincblende-type ZnX ($X = \text{S, Se, Te}$) compounds at room temperature

Compound	Element	Mean-Square Displacement (\AA^2)			
		SMM	Expt. ³⁴	Shell Model ¹⁵	<i>Ab Initio</i> ¹⁶
ZnS	Zn	0.0072	0.0111	0.0108	0.0102
	S	0.0075	0.0090	0.0093	0.0078
ZnSe	Zn	0.0106	0.0129	0.0125	0.0130
	Se	0.0106	0.0090	0.0084	0.0095
ZnTe	Zn	0.0132	0.0164	0.0169	0.0160
	Te	0.0131	0.0096	0.0121	0.0120

and other theoretical results for the atomic mean-square displacements is fairly good over the whole temperature region from 0 K to 600 K, much higher than the Debye temperature. The results presented herein confirm that the present SMM formalism can take into account quantum-mechanical zero-point vibrations as well as higher-order anharmonic terms in the atomic displacements.

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