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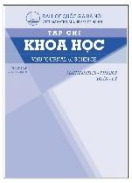

Original Article

Influence of Temperature and Pressure on the Lattice Constant of $SrTiO_3$ Perovskite by the Statistical Moment Method with Improved Interatomic Potential

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Abstract: Temperature and pressure dependence of lattice constants of a cubic Strontium Titanate ($SrTiO_3$) has been investigated using the statistical moment method. The lattice constants at various temperatures is derived in closed analytic form by including the anharmonic effects of the lattice vibrations explicitly. The potential with the partial charge model and Morse function is used. The numerical lattice constants at high temperatures by the statistical moment method are in good and reasonable agreement with the other theories and the experimental data. Variations of the lattice parameter of $SrTiO_3$ with the temperature are obtained at 1 atm, 8.2 GPa, and 15.2 GPa. Increasing of the lattice constants with increasing temperature is due to enhancing atomic anharmonic fluctuations in $SrTiO_3$ lattice crystal at higher temperature. A decrease of the lattice constants with increasing pressure can be demonstrated by the reduction of atomic vibrations in $SrTiO_3$ crystal lattice at higher pressures.

Keywords: Strontium Titanate, Lattice constant, Pressure, Statistical moment method, Anhammonicity.

1. Introduction

Strontium Titanate ($SrTiO_3$), a type-perovskite oxide, undergoes a sequence of phase transitions from cubic $\left(Pm\bar{3}m\right)$ to tetragonal $\left(I4/mcm\right)$, then to orthorhombic $\left(Cmcm\right)$ [1]. The cubic-tetragonal phase transition of $SrTiO_3$ dependents on temperature and pressure have been provided, such

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as at room temperature and the phase pressure of 9.6 GPa; at 381 K and 15.0 GPa, and 467 K and 18.7 GPa [2]. In the cubic phase with space group of $Pm\bar{3}m$, $SrTiO_3$ has a corner-linked anion octahedral TiO_6 with the Ti cations at the center of octahedra and the Sr cations in the space between the octahedra. $SrTiO_3$ cubic perovskite has a lattice constant of 3.905 A at room temperature [3, 4].

The understanding of $SrTiO_3$ is an active research field for the development of newly designed for different potential scientific and technological applications, such as gas sensors [5], fuel cells [6], and the substrate of superconductors [7]. In the design of the new material beyond $SrTiO_3$ material used stably in a wide temperature or at high temperatures, such as composite materials, their components must have consistent thermal properties, such as nearly and the same thermal expansion or lattice constant [8, 9]. The misfit of lattice parameter and the differences in the thermal expansion is original for altering the superconducting transition temperature of superconductors [10-12] and colossal magneto-resistance of films [13]. Thus, the variation of the lattice parameter of $SrTiO_3$ gave rise to a great deal of attention in theory [14-16] and experiment studies [3, 17-19].

With the same partial charge of ions in $SrTiO_3$ and only covalence bonding between Ti and O atoms, Seetawan et al., [15] could not reproduce the lattice parameter at high temperature in agreement with the experiment [14]. Otherwise, all studies from Katsumata [16], Seetawan [15], and Goh [14] used the Buckingham potential part, and this can be a problem for simulation at high temperatures [20-22].

To calculate lattice parameters of material with cubic structure at various temperatures, the statistical moment method (SMM) has been developed and successful for many types of crystal systems [23-27] with considering both the anharmonicity and quantum mechanical effects of the fluctuation in lattice crystal. In SMM, the Helmholtz free energies of crystals are derived in analytic form from the moment expansion technique in the quantum statistical mechanic, and the lattice parameter of materials are obtained from the explicit expressions in a wide range of temperature and pressure.

In this paper, it is the first time we have used SMM to determine mean-square atomic displacements and lattice constant of cubic $SrTiO_3$ at various temperatures and pressures. Using the effective pair potential between atoms with the partial charge model and Morse function, these quantities of $SrTiO_3$ are calculated numerically. The equation of state of $SrTiO_3$ is obtained from the Helmholtz free energy, which permits us to calculate the lattice parameter at various pressure within taking into account the anharmonicity effects of the thermal lattice vibrations. Furthermore, we will compare our calculation results with the previous theoretical calculations and the available experimental results.

2. Theory

2.1. Helmholtz Free Energy and the Equation of State of $SrTiO_3$

We will present the SMM formulation to calculate the Helmholtz free energy of $SrTiO_3$ for cubic SrTiO3, as schematically shown in Figure 1. Atoms Sr, Ti, and O are at the corner sites, the central site, at the centers of the cubic faces, respectively.

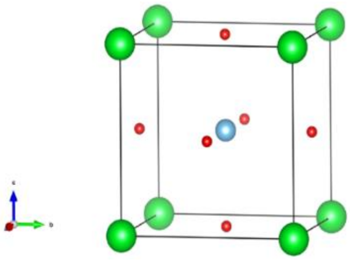

Figure 1. A unit cell of $SrTiO_3$ with a cubic structure.

Let us consider 5N atoms of cubic SrTiO3. A unit cell of $SrTiO_3$ has five atoms. Then we can calculate $N^{Sr}=N$ atoms Sr, $N^{Ti}=N$ atoms Ti, and $N^{O}=3N$ atoms O, and the concentration of Sr, Ti, and O atoms are $C_{Sr}=\frac{1}{5}$, $C_{Ti}=\frac{1}{5}$ and $C_O=\frac{3}{5}$, respectively.

The Helmholtz free energy of $SrTiO_3$ is given taking into account the configuration entropy of the system *Sc*, via the Boltzmann relation as [26]

$$\Psi = C_{Sr}\Psi^{Sr} + C_{Ti}\Psi^{Ti} + C_O\Psi^{O} - TS_c \tag{1}$$

Where Ψ^{Sr}, Ψ^{Ti} and Ψ^{O} present the Helmholtz free energy of Sr, Ti, and O ions, respectively.

Using moment expansion formulas [27], [28], the expressions of the partial Helmholtz free energies Ψ^{Sr}, Ψ^{Ti}, and Ψ^{O} in $SrTiO_3$ are given by

$$\begin{aligned}\Psi^{Sr} &= U_0^{Sr} + 3N^{Sr}\theta\left[x_{Sr}+\ln\left(1-e^{-2x_{Sr}}\right)\right]\\ &+3N^{Sr}\left\{\begin{array}{l}\dfrac{\theta^2}{\left(k^{Sr}\right)^2}\left[\gamma_2^{Sr}x_{Sr}^2cth^2x_{Sr}-\dfrac{2\gamma_1^{Sr}}{3}\left(1+\dfrac{x_{Sr}cthx_{Sr}}{2}\right)\right]\\ +\dfrac{2\theta^3}{\left(k^{Sr}\right)^4}\left[\dfrac{4}{3}\left(\gamma_2^{Sr}\right)^2x_{Sr}cthx_{Sr}\left(1+\dfrac{x_{Sr}cthx_{Sr}}{2}\right)-2\left(\left(\gamma_1^{Sr}\right)^2+2\gamma_1^{Sr}\gamma_2^{Sr}\right)\left(1+\dfrac{x_{Sr}cthx_{Sr}}{2}\right)(1+x_{Sr}cthx_{Sr})\right]\end{array}\right\}\end{aligned} \tag{2}$$

$$\begin{aligned}\Psi^{Ti} &= U_0^{Ti} + 3N^{Ti}\theta\left[x_{Ti}+\ln\left(1-e^{-2x_{Ti}}\right)\right]\\ &+3N^{Ti}\left\{\begin{array}{l}\dfrac{\theta^2}{\left(k^{Ti}\right)^2}\left[\gamma_2^{Ti}x_{Ti}^2cth^2x_{Ti}-\dfrac{2\gamma_1^{Ti}}{3}\left(1+\dfrac{x_{Ti}cthx_{Ti}}{2}\right)\right]\\ +\dfrac{2\theta^3}{\left(k^{Ti}\right)^4}\left[\dfrac{4}{3}\left(\gamma_2^{Ti}\right)^2x_{Ti}cthx_{Ti}\left(1+\dfrac{x_{Ti}cthx_{Ti}}{2}\right)-2\left(\left(\gamma_1^{Ti}\right)^2+2\gamma_1^{Ti}\gamma_2^{Ti}\right)\left(1+\dfrac{x_{Ti}cthx_{Ti}}{2}\right)(1+x_{Ti}cthx_{Ti})\right]\end{array}\right\}\end{aligned} \tag{3}$$

$$\begin{aligned}\Psi^{O} &= U_0^{O} + 3N^{O}\theta\left[x_{O}+\ln\left(1-e^{-2x_{O}}\right)\right]\\ &+3N^{O}\left\{\begin{array}{l}\dfrac{\theta^2}{\left(k^{O}\right)^2}\left[\gamma_2^{O}x_{O}^2cth^2x_{O}-\dfrac{2\gamma_1^{O}}{3}\left(1+\dfrac{x_{O}cthx_{O}}{2}\right)\right]\\ +\dfrac{2\theta^3}{\left(k^{O}\right)^4}\left[\dfrac{4}{3}\left(\gamma_2^{O}\right)^2x_{O}cthx_{O}\left(1+\dfrac{x_{O}cthx_{O}}{2}\right)-2\left(\left(\gamma_1^{O}\right)^2+2\gamma_1^{O}\gamma_2^{O}\right)\left(1+\dfrac{x_{O}cthx_{O}}{2}\right)(1+x_{O}cthx_{O})\right]\end{array}\right\}\end{aligned} ,\tag{4}$$

where

U_0^{Sr}, U_0^{Ti}, and U_0^{O} present the sum of effective pair interaction energies for Sr ion, Ti ion, and O ion, respectively. They are derived in the following form

$$U_0^{Sr}=\frac{N^{Sr}}{2}\sum_i\varphi_{i0}^{Sr}\left(|r_i|\right), U_0^{Ti}=\frac{N^{Ti}}{2}\sum_i\varphi_{i0}^{Ti}\left(|r_i|\right), U_0^{O}=\frac{N^{O}}{2}\sum_i\varphi_{i0}^{O}\left(|r_i|\right). \tag{5}$$

Harmonic parameters k^{Sr}, k^{Ti}, and k^{O}, anharmonic expansion coefficients γ_1^{Sr}, γ_1^{Ti}, γ_1^{O}, γ_2^{Sr}, γ_2^{Ti} and γ_2^{O} are determined by [27]

$$k^{Sr}=\frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{i0}^{Sr}}{\partial u_{i\alpha}^2}\right)_{eq},\ k^{Ti}=\frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{i0}^{Ti}}{\partial u_{i\alpha}^2}\right)_{eq};k^{O}=\frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{i0}^{O}}{\partial u_{i\alpha}^2}\right)_{eq} \tag{6}$$

$$\gamma_1^{Sr}=\frac{1}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{Sr}}{\partial u_{i\alpha}{}^4}\right)_{eq},\gamma_1^{Ti}=\frac{1}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{Ti}}{\partial u_{i\alpha}{}^4}\right)_{eq},\gamma_1^{O}=\frac{1}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{O}}{\partial u_{i\alpha}{}^4}\right)_{eq} \tag{7}$$

$$\gamma_2^{Sr}=\frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{Sr}}{\partial u_{i\alpha}{}^2\partial u_{i\beta}{}^2}\right)_{eq},\gamma_2^{Ti}=\frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{Ti}}{\partial u_{i\alpha}{}^2\partial u_{i\beta}{}^2}\right)_{eq},\gamma_2^{O}=\frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{O}}{\partial u_{i\alpha}{}^2\partial u_{i\beta}{}^2}\right)_{eq} \tag{8}$$

with $\alpha\neq\beta=x,y,$ or z, and

$$x_{Sr}=\frac{\hbar\omega_{Sr}}{2\theta};\omega_{Sr}=\sqrt{\frac{k^{Sr}}{m^*}},x_{Ti}=\frac{\hbar\omega_{Ti}}{2\theta};\omega_{Ti}=\sqrt{\frac{k^{Ti}}{m^*}},x_O=\frac{\hbar\omega_O}{2\theta};\omega_O=\sqrt{\frac{k^O}{m^*}}\ and\ \theta=k_BT \tag{9}$$

Here k_B is the Boltzmann constant, and m^* represents the average atomic mass being given by

$$m^*=C_{Sr}.m_{Sr}+C_{Ti}.m_{Ti}+C_O.m_O \tag{10}$$

Where m_{Sr}, m_{Ti}, and m_O are the atomic mass of Sr, Ti, and O atoms, respectively.

The results in (2)(3)(4) permit us to calculate the free energy at temperature T when the parameters k, γ_1 and γ_2 at T_0 are known. If the temperature T_0 is not far from T, then in assumption, the vibration of a particle is harmonic around a new equilibrium position (corresponding T_0). Therefore, Eqs. (2), (3) , and (4) can be rewritten by

$$\Psi^{Sr}=U_0^{Sr}+3N^{Sr}\theta\left[x_{Sr}+\ln\left(1-e^{-2x_{Sr}}\right)\right] \tag{11}$$

$$\Psi^{Ti}=U_0^{Ti}+3N^{Ti}\theta\left[x_{Ti}+\ln\left(1-e^{-2x_{Ti}}\right)\right] \tag{12}$$

$$\Psi^{O}=U_0^{O}+3N^{O}\theta\left[x_{O}+\ln\left(1-e^{-2x_{O}}\right)\right] \tag{13}$$

2.2. Calculating the Lattice Parameter of SrTiO$_3$

From the free energy Ψ, the pressure P can be determined by [27],

$$P=-\left(\frac{\partial\Psi}{\partial V}\right)_T=-\frac{r_1}{3V}\left(\frac{\partial\Psi}{\partial r_1}\right) \tag{14}$$

Using Eqs. (1), (11) - (14) for cubic SrTiO$_3$, we obtain an equation of the state of SrTiO$_3$ at zero temperature,

$$\begin{aligned}P&=-\frac{5}{24.r_1^2}\left(\frac{\partial\Psi}{\partial r_1}\right)_T\\&=-\frac{5}{24.r_1^2}\left\{C_{Sr}\left[\frac{1}{6}\frac{\partial U_0^{Sr}}{\partial r_1}+\frac{\hbar\omega_{Sr}}{4k^{Sr}}.\frac{\partial k^{Sr}}{\partial r_1}\right]+C_{Ti}\left[\frac{1}{6}\frac{\partial U_0^{Ti}}{\partial r_1}+\frac{\hbar\omega_{Ti}}{4k^{Ti}}.\frac{\partial k^{Ti}}{\partial r_1}\right]+C_O\left[\frac{1}{6}\frac{\partial U_0^{O}}{\partial r_1}+\frac{\hbar\omega_{O}}{4k^{O}}.\frac{\partial k^{O}}{\partial r_1}\right]\right\}\end{aligned} \tag{15}$$

The solution of the equation of state (15) is the value of the nearest-neighbor distance $r_1(P,0)$ between two intermediate atoms in $SrTiO_3$ lattice crystal at pressure P and zero temperature.

From the solution of Eq. (15) $r_1(P,0)$, we assume that the average nearest-neighbor distance between two atoms in $SrTiO_3$ at temperature T and pressure P, $r_1(P,\mathrm{T})$, can be written by

$$r_1(P,T)=r_1(P,0)+C_{Sr}.\mathrm{y}^{Sr}(P,T)+C_{Ti}.y^{Ti}(P,T)+C_O.y^O(P,T) \tag{16}$$

where $y^{Sr}(P,T)$, $y^{Ti}(P,T)$ and $y^O(P,T)$ are the displacements of the Sr, Ti, and O atoms from equilibrium position in the crystal lattice of $SrTiO_3$, respectively.

$y^{Sr}(P,T)$, $y^{Ti}(P,T)$ and $y^O(P,T)$ are calculated by

$$y^{Sr}=\sqrt{\frac{2\gamma^{Sr}\theta}{3\left(k^{Sr}\right)^3}A^{Sr}},\ y^{Ti}=\sqrt{\frac{2\gamma^{Ti}\theta}{3\left(k^{Ti}\right)^3}A^{Ti}},\ y^O=\sqrt{\frac{2\gamma^{O}\theta}{3\left(k^{O}\right)^3}A^{O}}, \tag{17}$$

where

$$\gamma^{Sr}=4\left(\gamma_1^{Sr}+\gamma_2^{Sr}\right),\gamma^{Ti}=4\left(\gamma_1^{Ti}+\gamma_2^{Ti}\right),\gamma^{O}=4\left(\gamma_1^{O}+\gamma_2^{O}\right). \tag{18}$$

And A^b (b = Sr, Ti, and O) are given by

$$A^b=a^b{}_1+\frac{\left(\gamma^b\right)^2\theta^2}{\left(k^b\right)^4}a_2^b+\frac{\left(\gamma^b\right)^3\theta^3}{\left(k^b\right)^6}a_3^b+\frac{\left(\gamma^b\right)^4\theta^4}{\left(k^b\right)^8}a_4^b+\frac{\left(\gamma^b\right)^5\theta^5}{\left(k^b\right)^{10}}a_5^b+\frac{\left(\gamma^b\right)^6\theta^6}{\left(k^b\right)^{12}}a_6^b$$

$$a_1^b=1+\frac{x_b cthx_b}{2},$$

$$a_2^b=\frac{13}{3}+\frac{47}{6}x_b cthx_b+\frac{23}{6}\left(x_b cthx_b\right)^2+\frac{1}{2}\left(x_b cthx_b\right)^3,$$

$$a_3^b=-\left(\frac{25}{3}+\frac{121}{6}x_b cthx_b+\frac{50}{3}\left(x_b cthx_b\right)^2+\frac{16}{3}\left(x_b cthx_b\right)^3+\frac{1}{2}\left(x_b cthx_b\right)^4\right),$$

$$a_4^b=\frac{43}{3}+\frac{93}{2}\left(x_b cthx_b\right)+\frac{169}{3}\left(x_b cthx_b\right)^2+\frac{83}{3}\left(x_b cthx_b\right)^3+\frac{22}{3}\left(x_b cthx_b\right)^4+\frac{1}{2}\left(x_b cthx_b\right)^5,$$

$$a_5^b=-\left(\begin{array}{l}\frac{103}{3}+\frac{749}{6}x_b cthx_b+\frac{363}{2}\left(x_b cthx_b\right)^2+\frac{391}{3}\left(x_b cthx_b\right)^3+\frac{148}{3}\left(x_b cthx_b\right)^4+\frac{53}{6}\left(x_b cthx_b\right)^5\\+\frac{1}{2}\left(x_b cthx_b\right)^6\end{array}\right),$$

$$\begin{aligned}a_6^b=65&+\frac{561}{2}\left(x_b cthx_b\right)+\frac{1489}{3}\left(x_b cthx_b\right)^2+\frac{927}{2}\left(x_b cthx_b\right)^3+\frac{733}{3}\left(x_b cthx_b\right)^4+\frac{145}{2}\left(x_b cthx_b\right)^5\\&+\frac{31}{3}\left(x_b cthx_b\right)^6+\frac{1}{2}\left(x_b cthx_b\right)^7.\end{aligned} \tag{19}$$

After deriving $r_1(P,\mathrm{T})$, we can calculate the lattice constant of $SrTiO_3$ as

$$a_c(P,T)=2r_1(P,T) \tag{20}$$

2.3. Interatomic Potential

In this paper, we use the form of the potential taken from combining Pedone’s form [21] and Demontis’s form [29]. It is given by

$$U(r_{ij}) = q_i q_j . \left\{ \frac{erfc(\alpha r_{ij})}{r_{ij}} - \frac{erfc(\alpha R_c)}{R_c} + \left[\frac{erfc(\alpha R_c)}{R_c^2} + \frac{2\alpha}{\pi^{\frac{1}{2}}} . \frac{erfc(-\alpha^2 R_c^2)}{R_c} \right] \left(r_{ij} - R_c \right) \right\} + D_{ij} \left[\left\{ 1 - e^{-\beta_{ij}(r_{ij} - r_o)} \right\}^2 - 1 \right] + \frac{C_{ij}}{r_{ij}^{12}} \quad (21)$$

where *i*, *j* present the type of ions: $i, j \in \{Sr, Ti, O\}$. R_c is the cutoff radius.

The first term describes the long-range Coulomb interaction between ions in $SrTiO_3$, where q_i and q_j are the effective charges of *i*-th and *j*-th intermolecular ions, and r_{ij} is the distance between them. The charges of ions Sr, Ti, and O are taken from the results presented by S. Piskunov et al. [30] and are given in Table 1.

Table 1. Potential parameters

Ion	q_i(e) [30]			
Sr	1.87			
Ti	2.36			
O	-1.41			
Ion pair	D_{ij}(eV)	β_{ij}(A^{-1})	r_{0ij}(A)	C_{ij}(eV.A^{12})
Sr - O	0.016561	2.191500	3.328330	3.0
Ti - O	0.021905	2.085525	2.708943	1.0
O - O	0.151000	1.081100	3.618701	22.0

In order the way minimizing the potential energy, we obtain the damping parameter α is 0.01(A^{-1}) and the cutoff radius R_c are 9.9145 (A), 9.7220 (A), and 9.7220 (A) for Sr, Ti, and O, respectively.

The second term presents the short-range Morse function of covalent bonds between the intermolecular ions in $SrTiO_3$ material. Where D_{ij} is the bond dissociation energy, β_{ij} is a function of the slope of the potential energy well, and r_{0ij} is the equilibrium bond distance. D_{ij}, β_{ij}, and r_{0ij} can be considered as parameters. These parameters have been obtained because they can reproduce the lattice parameter, thermal expansion, and heat capacity in good agreement with the experimental values of the thermodynamic quantities and are given in Table 1.

The last term represents repulsive contribution and adds to the interaction model at high temperature and pressure [21]. The parameters C_{ij} for interactions between pair-ions are also shown in Table 1.

3. Numerical Results and Discussions

To derive the numerical results of the thermodynamic quantities for $SrTiO_3$, we have taken the physical constants, including Boltzmann constant k_B, Plank constant $\hbar$, electric constant, and Avogadro constant Na from [31]. Applying the potential model (21) and the parameters in Table 1, we evaluate the parameters and the thermodynamic quantities of $SrTiO_3$ at the temperature T and pressure P by using the corresponding analytic expressions.

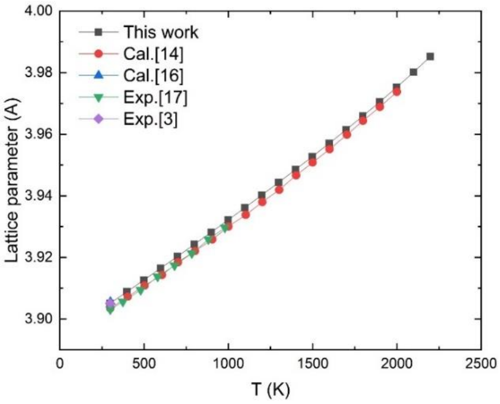

Figure 2. Temperature dependence of lattice parameter of $SrTiO_3$ at zero pressure.

From Eqs. (18) and (19), the anharmonic parameters are calculated within approximation up to the fourth-order of the power moments of the atomic displacements. Then substituting them on Eqs. (16), (17), and (20), the lattice parameter of $SrTiO_3$ is calculated in a wide range of temperatures from room temperature to 2198 K and shown in Figure 2 as a function of temperature. Our result matches very well with experimental [3, 17] and calculated results [14, 16] in the wide temperature range from room temperature up to high temperature. As it can be seen from Figure 2, the lattice parameter increases with increasing temperature. This effect can be explained by enhancing atomic anharmonic fluctuations in $SrTiO_3$ lattice crystal when temperature increases. When temperature increases from room temperature to 2198 K, the lattice constant increases by about 8.0%, and the slope of the curve is about $\left|da_c / dT\right| \approx 0.00096 - 0.00128 (A / K)$. This result implies that the lattice constant of $SrTiO_3$ is a nonlinear function of temperature.

To consider the effects of pressure on the lattice constant, we solve Eq. (15) and use Eq. (20) to calculate the lattice parameter of $SrTiO_3$ at the various values of temperature and pressure.

The pressure-induced lattice parameters at various temperatures are calculated and are shown in Figures 3-5.

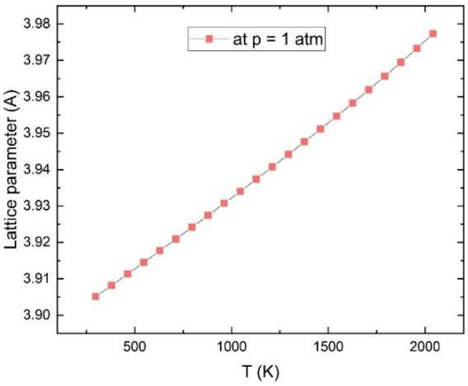

Figure 3. Variation of the lattice parameter of $SrTiO_3$ with the temperature at 1 atm.

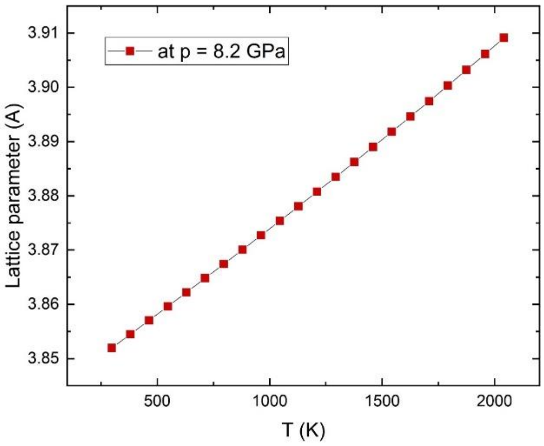

Figure 4. Variation of the lattice parameter of $SrTiO_3$ with the temperature at 8.2GPa.

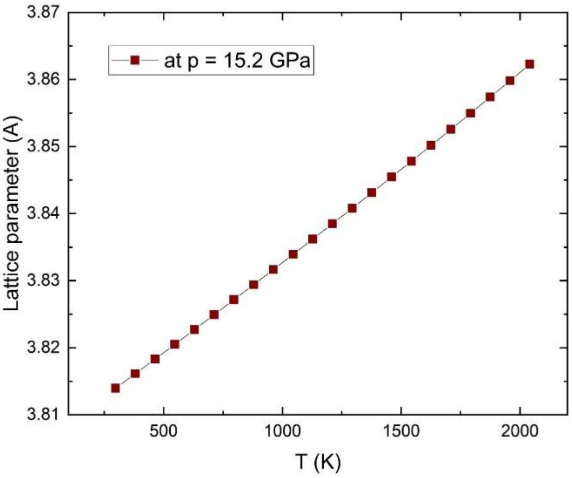

Figure 5. Variation of the lattice parameter of $SrTiO_3$ with the temperature at 15.2GPa.

In Figures. 3-5, pressure increases from 1 atm up to 15.2 GPa, and the lattice constant increases with temperature in a wide temperature from 298 K to 2041 K. So it can be seen from Figures. 3-5, the lattice constants of $SrTiO_3$ are the decreasing functions of pressure and the increasing function of temperature. This effect can be demonstrated by the reduction of atomic vibrations in $SrTiO_3$ crystal lattice when pressure increases.

4. Conclusion

In the present work, we firstly apply the statistical moment method in quantum statistical mechanics to investigate the pressure temperature-dependence of the lattice parameter of cubic $SrTiO_3$ perovskite in a wide temperature and pressure range. The lattice constant at various temperatures and pressures is derived in closed analytic form by including the anharmonic effects of the lattice vibrations explicitly. We have combined the potential forms published by Pedone and Demontis to obtain the lattice parameter of $SrTiO_3$ perovskite in agreement with the experiment in a wide temperature range. Increasing of the lattice parameter with temperature is due to enhancing atomic anharmonic fluctuations in $SrTiO_3$ lattice crystal when temperature increases. Decreasing the lattice parameter with increasing pressure can be demonstrated by the reduction of atomic vibrations in $SrTiO_3$ crystal lattice when pressure increases.

In a good and reasonable agreement between our calculated results with experimental measurements and those of the other theoretical calculations imply the efficiency of the statistical moment method in investigating the temperature dependence on thermodynamic quantities of materials. The advantage of this approach compared to other theoretical methods is that it has considered the higher-order anharmonic terms in the atomic displacements and the quantum-mechanical zero-point vibrations. Therefore, it has a great potential to be developed to study the temperature and pressure effects on the thermodynamic properties of the other perovskite materials.

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