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STUDY OF TEMPERATURE AND PRESSURE EFFECTS ON THE LATTICE PARAMETER OF CUBIC $BaTiO_3$ BY THE STATISTICAL MOMENT METHOD WITH IMPROVED INTERATOMIC POTENTIAL PARAMETERS

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Abstract. The effects of temperature and pressure on the lattice parameter of barium titanate with cubic structure have been studied by the statistical moment method. The analytic expression of the lattice parameter is obtained by considering the anharmonic lattice vibrations. The potential with their improved parameters is used to obtain the lattice parameters of $BaTiO_3$ from 400 K up to 1500 K and from zero up to 11 GPa. The numerical lattice parameters at various temperatures and pressures are consistent with the experimental result. The lattice parameter changes as a decreased function of the pressure but an increased function of the temperature.
Keywords: $BaTiO_3$, lattice parameter, statistical moment method, anharmmonicity.

1. Introduction

$BaTiO_3$ is a typical perovskite oxide ABO_3. It has taken more attention and application, such as a capacitor dielectric [1], a non-volatile ferroelectric random access memory (FeRAM) [2], and energy storage [3]. With changing pressure or temperature, $BaTiO_3$ can take the phase transitions ranging from the high-symmetry cubic phase ($Pm\bar{3}m$) to tetragonal (*P4mm*), orthorhombic (*Amm2*), and rhombohedral (*R3m*) ones in nature [4, 5]. The phase transition of $BaTiO_3$ from cubic structure to tetragonal at various conditions of pressure and temperature, such as at zero pressure and 393 K [6], at zero temperature, and 6.5 GPa [4] Cubic $BaTiO_3$ has a space group $Pm\bar{3}m$ and a lattice constant of 3.996 $\mathring{A}$ at 120^{o}C [7].

When designing a novel material from $BaTiO_3$, their thermal properties have to be consistent with $BaTiO_3$, such as similar thermal expansion or lattice parameters [8]. The differences in the lattice constant and the thermal expansion can be original to alter the superconducting transition temperature of superconductors [9-11]. Thus, the change of the lattice parameter of $BaTiO_3$ has much attention in theoretical [12, 13] and experimental research [4, 7, 8].

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In $BaTiO_3$, some literature presented that the formal charge of Ba, Ti, and O ions are +2, +4, and -2, respectively. However, many studies, such as [14], have shown that the ions in $BaTiO_3$ possess fractional charges. In [15] and [16], we have applied the partial charge model for $SrTiO_3$ perovskite, which has a similar perovskite structure and atomic bonding with $BaTiO_3$. The results suggest that we can continue using the partial charge mode for $BaTiO_3$ perovskite.

In recent years, the statistical moment method (SMM) have gotten successful in studying the thermodynamic properties of crystal material with cubic structure [17-21]. SMM considers both the anharmonic and quantum effects in lattice crystals. Significantly, the authors in [15] and [16] have shown a good agreement between the SMM calculation with the experiment studies for cubic $SrTO_3$, a kind of perovskite with a structure like cubic $BaTiO_3$.

In this study, we use SMM considering the fourth-order moment of the atomic displacements to discover the lattice parameters of cubic $BaTiO_3$ at different temperatures and pressure. We will continue using the interatomic potential form with the partial charge of the atoms used in [15, 16] to obtain the numerical results for cubic $BaTiO_3$.Then, our calculation will be compared with the various theory and experiment research.

2. Content

2.1. Helmholtz free energy of $BaTiO_3$

A unit cell of cubic $BaTiO_3$ is schematically shown in Figure 1.

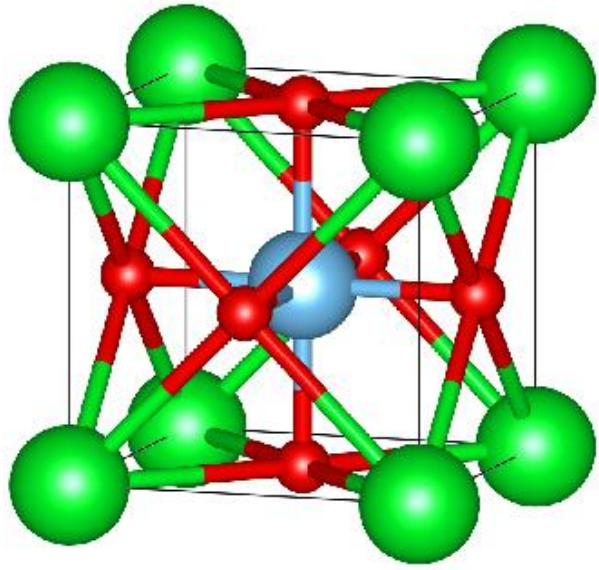

Figure 1. A unit cell of cubic $BaTiO_3$

It is shown that there are one atom Sr, one atom Ti and three atoms O in a unit cell. The atom Ba is located at the corner site and the atom Ti is the central site. The atoms O are at the central sites of the cubic faces. Then, the concentrations of three kinds of atoms are $C_{\mathrm{Sr}} = \frac{1}{5}$, $C_{\mathrm{Ti}} = \frac{1}{5}$ and $C_{\mathrm{O}} = \frac{3}{5}$ for Ba, Ti and O, respectively.

The Helmholtz free energy of $BaTiO_3$ can be expanded via the Boltzmann relation as follows [15, 20]:

$$\Psi = C_{\mathrm{Ba}}\Psi^{\mathrm{Ba}} + C_{\mathrm{Ti}}\Psi^{\mathrm{Ti}} + C_{\mathrm{O}}\Psi^{\mathrm{O}} - TS_c, \quad (1)$$

where Ψ^{p} (p = Ba, Ti, O) is the partial Helmholtz free energy of ion p.

From moment expansion formulas [15, 21, 22], the expressions of Ψ^{p} in $BaTiO_3$ have the form

$$\Psi^{p} = U_0^{p} + 3N^{p}\theta\left[x_p + \ln\left(1-e^{-2x_p}\right)\right] + 3N^{p}\left\{\frac{\theta^2}{\left(k^{p}\right)^2}\left[\gamma_2^{p}x_p^2 coth^2 x_p - \frac{2\gamma_1^{p}}{3}\left(1+\frac{x_p cothx_p}{2}\right)\right] + \right.$$

$$\left. + \frac{2\theta^3}{\left(k^{p}\right)^4}\left[\frac{4}{3}\left(\gamma_2^{p}\right)^2 x_p cothx_p\left(1+\frac{x_p cothx_p}{2}\right) - 2\left(\left(\gamma_1^{p}\right)^2 + 2\gamma_1^{p}\gamma_2^{p}\right)\left(1+\frac{x_p cothx_p}{2}\right)(1+x_p cothx_p)\right]\right\}, \tag{1}$$

where U_0^{p} is the sum of effective pair interaction energy for ion p. The expressions of U_0^{p} respectively for Ba, Ti and O are

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

The harmonic parameters k^{Ba}, k^{Ti} and k^{O}, the anharmonic expansion coefficients γ_1^{Ba}, γ_1^{Ti}, γ_1^{O}, γ_2^{Ba}, γ_2^{Ti} and γ_2^{O} are determined by [21]

$$k^{Ba} = \frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{i0}^{Ba}}{\partial u_{i\alpha}^2}\right)_{eq}, \ k^{Ti} = \frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{i0}^{Ti}}{\partial u_{i\alpha}^2}\right)_{eq}; k^{O} = \frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{i0}^{O}}{\partial u_{i\alpha}^2}\right)_{eq}, \tag{3}$$

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

$$\gamma_2^{Ba} = \frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{Ba}}{\partial u_{i\alpha}{}^2\partial u_{i\beta}{}^2}\right)_{eq}, \gamma_2^{Ti} = \frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{Ti}}{\partial u_{i\alpha}{}^2\partial u_{i\beta}{}^2}\right)_{eq}, \gamma_2^{O} = \frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{i0}^{O}}{\partial u_{i\alpha}{}^2\partial u_{i\beta}{}^2}\right)_{eq} \tag{5}$$

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

$$x_{Ba} = \frac{\hbar\omega_{Ba}}{2\theta}; \omega_{Ba} = \sqrt{\frac{k^{Ba}}{m^*}}, x_{Ti} = \frac{\hbar\omega_{Ti}}{2\theta}; \omega_{Ti} = \sqrt{\frac{k^{Ti}}{m^*}}, x_{O} = \frac{\hbar\omega_{O}}{2\theta}; \omega_{O} = \sqrt{\frac{k^{O}}{m^*}} \text{ and } \theta = k_B T \ . \tag{6}$$

Here k_B is the Boltzmann constant, m^* is the average atomic mass and is determined by

$$m^* = C_{Ba}m_{Ba} + C_{Ti}m_{Ti} + C_{O}m_{O}, \tag{7}$$

where m_{Ba}, m_{Ti} and m_{O} are the atomic mass of Ba, Ti, and O atoms, respectively.

The eq. allows computing Ψ^{p} at temperature T when the parameters k^{p}, γ_1^{p}, γ_2^{p} at T_0 are known. As T_0 is near T, in assumption, the atoms fluctuate harmonically about a new equilibrium position and the eq.(1) for Ba, Ti and O ions can be rewritten by

$$\Psi^{Ba} = U_0^{Ba} + 3N^{Ba}\theta\left[x_{Ba} + \ln\left(1-e^{-2x_{Ba}}\right)\right], \tag{8}$$

$$\Psi^{\mathrm{Ti}} = U_0^{\mathrm{Ti}} + 3N^{\mathrm{Ti}}\theta\left[x_{\mathrm{Ti}} + \ln\left(1-e^{-2x_{\mathrm{Ti}}}\right)\right], \tag{9}$$

$$\Psi^{\mathrm{O}} = U_0^{\mathrm{O}} + 3N^{\mathrm{O}}\theta\left[x_{\mathrm{O}} + \ln\left(1-e^{-2x_{\mathrm{O}}}\right)\right].. \tag{10}$$

2.2. Equation of state and the lattice parameter of $BaTiO_3$

The free energy Ψ is related to the pressure P by

$$P = -\left(\frac{\partial\Psi}{\partial V}\right)_T = -\frac{r_1}{3V}\left(\frac{\partial\Psi}{\partial r_1}\right). \tag{11}$$

Applying equations (8) for cubic $BaTiO_3$, at $T = 0K$, the equation of the state of $BaTiO_3$ is achieved in the following form

$$P = -\frac{5}{24.r_1^2}\left(\frac{\partial\Psi}{\partial r_1}\right)_T =$$

$$= -\frac{5}{24r_1^2}\left\{C_{\mathrm{Ba}}\left[\frac{1}{6}\frac{\partial U_0^{\mathrm{Ba}}}{\partial r_1} + \frac{\hbar\omega_{\mathrm{Ba}}}{4k^{\mathrm{Ba}}}.\frac{\partial k^{\mathrm{Ba}}}{\partial r_1}\right] + C_{\mathrm{Ti}}\left[\frac{1}{6}\frac{\partial U_0^{\mathrm{Ti}}}{\partial r_1} + \frac{\hbar\omega_{\mathrm{Ti}}}{4k^{\mathrm{Ti}}}.\frac{\partial k^{\mathrm{Ti}}}{\partial r_1}\right] + C_{\mathrm{O}}\left[\frac{1}{6}\frac{\partial U_0^{\mathrm{O}}}{\partial r_1} + \frac{\hbar\omega_{\mathrm{O}}}{4k^{\mathrm{O}}}.\frac{\partial k^{\mathrm{O}}}{\partial r_1}\right]\right\}. \tag{12}$$

The equation (12) permits us to obtain the interatomic nearest-neighbor distance $r_1(P,0)$ in $BaTiO_3$ at pressure P and zero temperature. Then**,** in assumption, the average interatomic nearest-neighbor distance at temperature T and pressure P, $r_1(P,\mathrm{T})$, is given by

$$r_1(P,T) = r_1(P,0) + C_{\mathrm{Ba}}y^{\mathrm{Ba}}(P,T) + C_{\mathrm{Ti}}y^{\mathrm{Ti}}(P,T) + C_{\mathrm{O}}.y^{\mathrm{O}}(P,T), \tag{13}$$

where $y^p(P,T)$ are the displacements of the atom p from the equilibrium position. From [21], the expressions of $y^p(P,T)$ for Ba, Ti, and O atoms have the form

$$y^{\mathrm{Ba}} = \sqrt{\frac{2\gamma^{\mathrm{Ba}}\theta}{3\left(k^{\mathrm{Ba}}\right)^3}A^{\mathrm{Ba}}}, y^{\mathrm{Ti}} = \sqrt{\frac{2\gamma^{\mathrm{Ti}}\theta}{3\left(k^{\mathrm{Ti}}\right)^3}A^{\mathrm{Ti}}}, y^{\mathrm{O}} = \sqrt{\frac{2\gamma^{\mathrm{O}}\theta}{3\left(k^{\mathrm{O}}\right)^3}A^{\mathrm{O}}}, \tag{14}$$

where

$$\gamma^{\mathrm{Ba}} = 4\left(\gamma_1^{\mathrm{Ba}} + \gamma_2^{\mathrm{Ba}}\right), \gamma^{\mathrm{Ti}} = 4\left(\gamma_1^{\mathrm{Ti}} + \gamma_2^{\mathrm{Ti}}\right), \gamma^{\mathrm{O}} = 4\left(\gamma_1^{\mathrm{O}} + \gamma_2^{\mathrm{O}}\right) \tag{15}$$

and A^p (p = Ba, Ti, and O) are given by

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

$$a_1^p = 1 + \frac{X_p}{2}, a_2^p = \frac{13}{3} + \frac{47}{6}X_p + \frac{23}{6}X_p^2 + \frac{1}{2}X_p^3, a_3^p = -\left(\frac{25}{3} + \frac{121}{6}X_p + \frac{50}{3}X_p^2 + \frac{16}{3}X_p^3 + \frac{1}{2}X_p^4\right),$$

$$a_4^p = \frac{43}{3} + \frac{93}{2}X_p + \frac{169}{3}X_p^2 + \frac{83}{3}X_p^3 + \frac{22}{3}X_p^4 + \frac{1}{2}X_p^5,$$

$$a_5^p = -\left(\frac{103}{3} + \frac{749}{6}X_p + \frac{363}{2}X_p^2 + \frac{391}{3}X_p^3 + \frac{148}{3}X_p^4 + \frac{53}{6}X_p^5 + \frac{1}{2}X_p^6\right),$$

$$a_6^p = 65 + \frac{561}{2}X_p + \frac{1489}{3}X_p^2 + \frac{927}{2}X_p^3 + \frac{733}{3}X_p^4 + \frac{145}{2}X_p^5 + \frac{31}{3}X_p^6 + \frac{1}{2}X_p^7, X_p \equiv x_p\coth x_p. \tag{17}$$

From that, the lattice constant of $BaTiO_3$ at pressure P and temperature T can be computed by

$$a_c(P,T) = 2r_1(P,T). \tag{16}$$

2.3. Interatomic potential

To calculate the potential energy for $BaTiO_3$, we continue the model of the following potential [15]

$$U(r_{ij}) = q_i q_j \cdot \left\{ \frac{erfc(\alpha r_{ij})}{r_{ij}} - \frac{erfc(\alpha R_c)}{R_c} + \left[\frac{erfc(\alpha R_c)}{R_c^2} + \frac{2\alpha}{\pi^{\frac{1}{2}}} \cdot \frac{erfc(-\alpha^2 R_c^2)}{R_c} \right] \left(r_{ij} - R_c \right) \right\} +$$
$$+ D_{ij} \left[\left\{ 1 - e^{-\beta_{ij}(r_{ij} - r_o)} \right\}^2 - 1 \right] + \frac{C_{ij}}{r_{ij}^{12}}, \tag{17}$$

where i, j display the type of ions, $i, j = \mathrm{Ba, Ti, O}$ and R_c is the cut-off radius.

The values of charge q_i and parameters D_{ij}, β_{ij}, r_{0ij} and C_{ij} for Ba, Ti, and O are given in Table 1 [14].

Table 1. Potential parameters for $BaTiO_3$

Ion	$q_i\,(\mathrm{e})$ [14]			
Ba	1.79			
Ti	2.38			
O	-1.39			
Ion pair	$D_{ij}\,(\mathrm{eV})$	$\beta_{ij}\left(\left(\mathrm{\AA}\right)^{-1}\right)$	$r_{0ij}\,(\mathrm{\AA})$	$C_{ij}\left(\mathrm{eV}.(\mathrm{\AA})^{12}\right)$
Ba - O	0.019561	2.071500	3.393410	5.0
Ti - O	0.021905	2.085525	2.708943	1.0
O - O	0.181000	1.098500	3.618701	22.0

We obtain the damping parameter $\alpha = 0.01\left(\left(\mathrm{\AA}\right)^{-1}\right)$, and the cut-off radius R_c = 10.1468 $(\mathrm{\AA})$, 9.9499 $(\mathrm{\AA})$ and 9.9499 $(\mathrm{\AA})$ for Ba, Ti, and O, respectively.

2.4. Numerical results and discussions

To calculate the thermodynamic quantities for BaTiO3 numerically, we use the physical constants from [23]. Then, applying the potential model (17) and its parameters, we compute the lattice parameter of $BaTiO_3$ from their corresponding expressions.

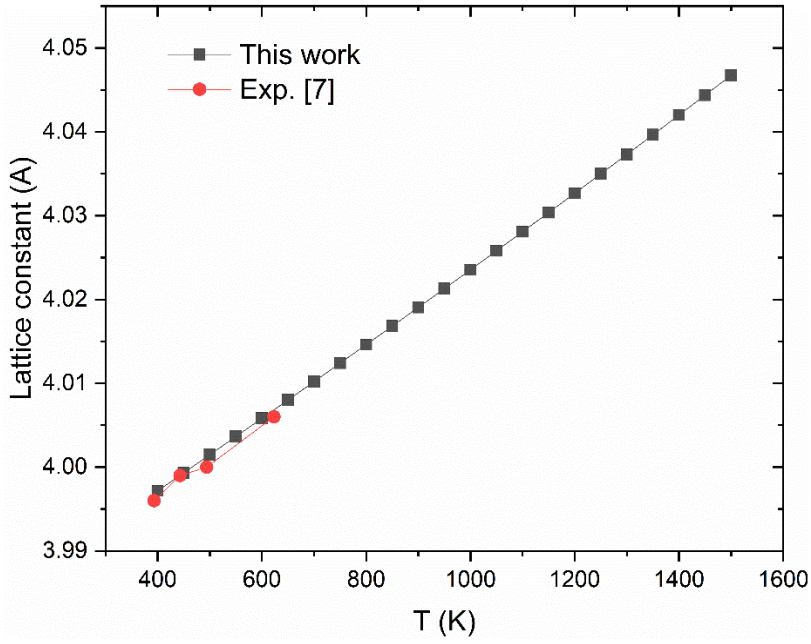

Figure 2. The lattice constant of $BaTiO_3$ as a function of temperature at zero pressure

From the equations (3), (4), (5), and (15), the harmonic and anharmonic parameters k^p, γ_1^p, γ_2^p are computed. Then apply them to the equations (14), (13) and (16), the lattice constant a_c of $BaTiO_3$ is derived from 400 K to 1500 K and shown in Figure 2. As can be seen from Figure 2, there is a good match between the two results. The lattice constant is an increasing function of temperature. This result is due to the enhancement of the anharmonic vibrations in $BaTiO_3$ as temperature raises. In the temperature range from 400 K to 1500 K, the lattice constant goes up by about 1.2% and the slope of the curve is about $\left|\frac{da_c}{dT}\right| \simeq 0.043 - 0.047\left(\text{Å}/\text{K}\right)$. That is shown that the lattice constant of $BaTiO_3$ increases nonlinearly with temperature.

To find out the change of the lattice constant as the pressure alters, we make the solution of the equations (12) at the different pressure values and zero temperature. Then, substituting that solution into the equation (16) we can derive the lattice parameter of $BaTiO_3$, a_c (P,T). The obtained lattice parameters of $BaTiO_3$ at pressures 3GPa, 5GPa, and 7 GPa, and in a temperature range from 400 K to 1000 K are shown in Figures 3 and 4.

Figure 3 shows that the lattice constant of $BaTiO_3$ decreases as pressure increases but increases when temperature decreases. This result implies that pressure and temperature affect the lattice parameter of $BaTiO_3$ oppositely.

In addition, Figure 4 shows more clearly the decrease of the lattice parameter in the pressure range from 3 GPa to 11 GPa. This result is caused by reducing atomic fluctuations in $BaTiO_3$ as pressure rises.

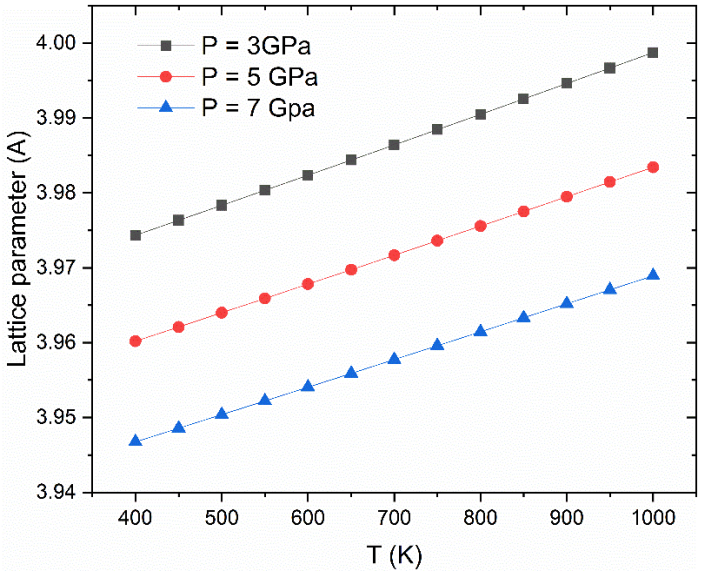

Figure 3. Temperature dependence of the lattice parameter of $BaTiO_3$ at 3 GPa, 5 GPa and 7 GPa

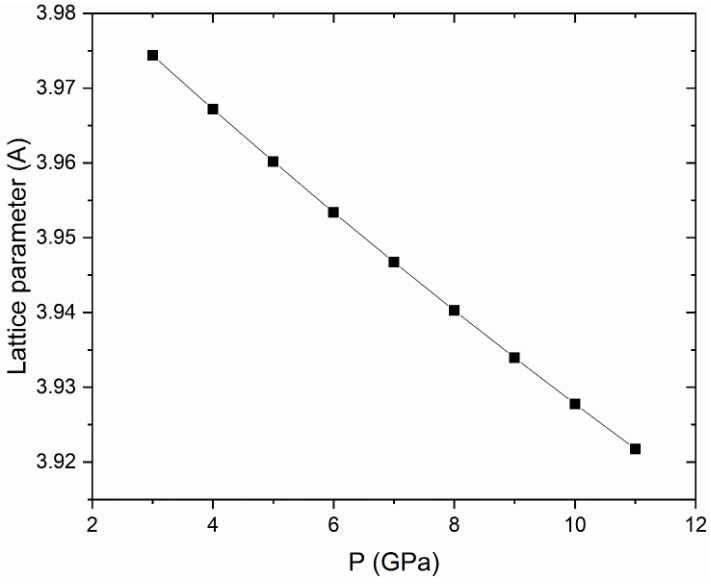

Figure 4. Pressure dependence of the lattice parameter for $BaTiO_3$ at 400 K

3. Conclusions

In this study, we perform SMM calculations to research the temperature-pressure dependence of lattice parameters for cubic $BaTiO_3$. The interatomic interaction potential model (17) with the improved parameters that we have used in [20, 21] continuously permits deriving the lattice parameter of cubic $BaTiO_3$ from 400 K to 1500 K and from zero up to 11GPa.

Atomic fluctuations in $BaTiO_3$ reduce when the pressure increases but it enhances as temperature increases. Therefore, the lattice parameter is a decreasing function of pressure and an increasing function of temperature.

The calculated lattice parameter by SMM has matched well with the experimental data. That implies that SMM efficiently investigates the temperature and pressure effects on the lattice parameter of cubic $BaTiO_3$. In advantage, SMM can be applied to investigate the temperature and pressure dependence of the thermodynamic quantities of cubic $BaTiO_3$.

REFERENCES

[1] A. M. G. Malcolm E. Lines, 1997. *Principles and applications of ferroelectrics and related materials*. Clarendon Press - Oxford.

[2] J. F. Seott, 2000. *Ferroelectric Memories. Springer Series in Advanced Microelectronics*, Vol. 3. Springer-Verlag Berlin Heidelberg.

[3] J. C. Liang Chen, Feng Li, Botao Gao, Chang Zhou, Jie Wu, Shiqing Deng, Hui Liu, He Qi, 2023. Excellent energy storage and mechanical performance in hetero-structure $BaTiO_3$-based relaxors. *Chem. Eng. J.*, Vol. 452, pp. 139222.

[4] T. Ishidate, S. Abe, H. Takahashi, and N. Mori, 1997. Phase Diagram of $BaTiO_3$. *Phys. Rev. Lett.*, Vol. 78, Iss. 12, pp. 2397–2400.

[5] J. Íñiguez and D. Vanderbilt, 2002. First-Principles Study of the Temperature-Pressure Phase Diagram of $BaTiO_3$. *Phys. Rev. Lett.*, Vol. 89, Iss. 11, pp. 9–12.

[6] G. A. Samara, 1966. Pressure and temperature dependences on the dielectric properties of the perovskites $BaTiO_3$ and $SrTiO_3$. *Phys. Rev.*, Vol. 151, Iss. 2, pp. 378-386.

[7] S. Miyake and R. Ueda, 1947. On Phase Transformation of $BaTiO_3$. *J. Phys. Soc. Japan*, Vol. 2, Iss. 5, pp. 93-97.

[8] P. Mirzadeh Vaghefi, A. Baghizadeh, M. Willinger, A. A. C. S. Lourenço, and V. S. Amaral, 2017. Effect of lattice mismatch on the magnetic properties of nanometer-thick $La_{0.9}Ba_{0.1}MnO_3$ (LBM) films and LBM/$BaTiO_3$/LBM heterostructures. *Appl. Surf. Sci.*, Vol. 425, pp. 988-995.

[9] H. Sato and M. Naito, 1997. Increase in the superconducting transition temperature by anisotropic strain effect in (001) $La_{1.85}Sr_{0.15}CuO_4$ thin films on $LaSrAlO_4$ substrates. *Phys. C Supercond. its Appl.*, Vol. 274, Iss. 3-4, pp. 221-226.

[10] J. P. Locquet, J. Perret, J. Fompeyrine, E. Mächler, J. W. Seo, and G. Van Tendeloo, 1998. Doubling the critical temperature of $La_{1.9}Sr_{0.1}CuO_4$ using epitaxial strain. *Nature*, Vol. 394, Iss. 6692, pp. 453-456.

[11] J.-S. Zhou, J. B. Goodenough, H. Sato, and M. Naito, 1999. Optimal superconductivity in $La_{2-x}Sr_xCuO_4$. *Phys. Rev. B*, Vol. 59, Iss. 5, pp. 3827-3830.

[12] R. Choithrani, 2014. Structural , Elastic and Thermal Properties of $BaTiO_3$. *Invertis J. Sci. Technol.*, Vol. 7, Iss. 2, pp. 72-77.

[13] P. Pruzan, D. Gourdain, J. C. Chervin, B. Canny, B. Couzinet, and M. Hanfland, 2002. Equation of state of $BaTiO_3$ and $KNbO_3$ at room temperature up to 30 GPa. *Solid State Commun.*, Vol. 123, Iss. 1-2, pp. 21-26.

[14] S. Piskunov, E. Heifets, R. I. Eglitis, and G. Borstel, 2004. Bulk properties and electronic structure of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ perovskites: An ab initio HF/DFT study. *Comput. Mater. Sci.*, Vol. 29, Iss. 2, pp. 165-178.

[15] C. H. Phuong and V. Van Hung, 2022. Study of the thermodynamic properties of $SrTiO_3$ perovskite by the statistical moment method with improved interatomic potential. *Mater. Today Commun.*, Vol. 31, Iss. 3, pp. 103439.

[16] C. H. Phuong and V. Van Hung, 2022. Study of the thermodynamic properties of $SrTiO_3$ perovskite under pressure by the statistical moment method with the improved interatomic potential. *Comput. Condens. Matter*, Vol. 31, Iss. 2, e00683.

[17] V. T. T. Ha, V. Van Hung, P. T. M. Hanh, N. V. Tuyen, T. T. Hai, and H. K. Hieu, 2016. Investigation of thermodynamic and mechanical properties of $Al_yIn_{1-y}P$ alloys by statistical moment method. *Phys. B Condens. Matter*, Vol. 532, Iss.12, pp. 76-79.

[18] V. V Hung, K. Masuda-Jindo, P. D. Tam, and S. R. Nishitani, 2001. Calculation of thermodynamic quantities of metals and alloys by the statistical moment method. *J. Phase Equilibria*, Vol. 22, Iss. 4, pp. 400-405.

[19] K. Masuda-Jindo, V. Van Hung, and P. E. A. Turchi, 2008. Application of statistical moment method to thermodynamic properties and phase transformations of metals and alloys. *Solid State Phenom.*, Vol. 138, Iss. 7, pp. 209-240.

[20] V. Van Hung, J. Lee, and K. Masuda-Jindo, 2006. Investigation of thermodynamic properties of cerium dioxide by statistical moment method. *J. Phys. Chem. Solids*, Vol. 67, Iss. 4, pp. 682-689.

[21] N. Tang and V. van Hung, 1988. Investigation of the Thermodynamic Properties of Anharmonic Crystals by the Momentum Method. I. General Results for Face-Centred Cubic Crystals. *Phys. Status Solidi*, Vol. 149, Iss. 2, pp. 511-519.

[22] K. Masuda-Jindo, V. Van Hung, and P. D. Tam, 2003. Thermodynamic quantities of metals investigated by an analytic statistical moment method. *Phys. Rev. B*, Vol. 67, Iss. 9, pp. 32-40.

[23] P. J. Mohr, D. B. Newell, and B. N. Taylor, 2016. CODATA recommended values of the fundamental physical constants: 2014. *Rev. Mod. Phys.*, Vol. 88, Iss. 3, pp. 1-73.