Analysis of the anharmonic thermal expansion coefficient of crystalline silver

Tong Sy Tien[1*], Nguyen Thi Minh Thuy[1], Nguyen Thi Viet Chinh[2],
Nguyen Cong Toan[3], Nguyen Bao Trung[3], Nguyen Van Nghia[4]

[1]Faculty of Fundamental Sciences, University of Fire Prevention & Fighting;
[2]Institute of Science and Technology, TNU-University of Sciences;
[3]Department of Physics, Hanoi University of Science;
[4]Faculty of Energy, Thuyloi University.
[*]Corresponding author: tongsytien@yahoo.com

Received 18 May 2023; Revised 10 Jul. 2023; Accepted 8 Aug. 2023; Published 25 Aug. 2023.
DOI: https://doi.org/10.54939/1859-1043.j.mst.89.2023.103-109

ABSTRACT

The anharmonic thermal expansion (TE) coefficient of crystalline silver (Ag) has been calculated and analyzed in the temperature-dependent. Based on the anharmonic effective potential, the calculation model is developed using the correlated Debye model and the many-body perturbation approach. Thermodynamic parameters of the crystal lattice are derived from the influence of thermal vibrations of all atoms. The anharmonicity results from phonon-phonon interactions, with each thermal vibration can be quantized and treated as a phonon. The obtained expression of the anharmonic TE coefficient of Ag can satisfy all their temperature-dependent fundamental properties. The numerical results of Ag agree well with those obtained from the other theoretical models and experimental data at various temperatures in the range from 0 K to 1000 K. The obtained results indicate the effectiveness of the present model in investigating the TE coefficient of Ag.

Keywords: Anharmonic thermal expansion coefficient; Crystalline silver; Anharmonic correlated Debye model.

1. INTRODUCTION

Nowadays, the anharmonic TE coefficient of metals can be measured experimentally with high precision and is one of the independent thermodynamic properties [1]. Like the heat capacity and compressibility, many dynamic properties of metals can be defined from their anharmonic TE coefficient [2], so accurate information about the temperature-dependent thermal expansion (TE) coefficient of metals is necessary and important in engineering physics, especially for metallurgy and mechanics [3]. However, thermal vibrations cause anharmonic effects [4] that change the interatomic distances of atoms and their positions in the crystal lattice [5]. Hence, the increasing temperature is sensitive to the anharmonic TE coefficient [6], as seen in Fig. 1.

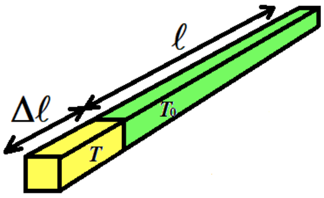

Figure 1. *Thermal expansion of metals with a temperature change.*

Hitherto, crystalline silver (Ag) has a face-centered cubic (FCC) structure, which is valued as a precious metal [7]. It can make jewels, brazing alloys, dental alloys, and mirrors and is used to produce batteries, electrical contacts, and antibacterial properties [8]. Moreover, Ag nanoparticles can prevent bacteria from forming unpleasant odors and digesting sweat [9].

In recent years, a quantum anharmonic correlated Einstein (QACE) model can calculate the anharmonic TE coefficient of metals even in the low-temperature (LT) region [10, 11], but it cannot mimic the acoustic phonon branches [12, 13]. Meanwhile, the classical anharmonic correlated Einstein (CACE) model has the advantage that the obtained expressions are simple in the dependent temperature [14]. Still, it is valid only in the high-temperature (HT) region [15].

Recently, an anharmonic correlated Debye (ACD) model has been used to effectively treat the anharmonic TE coefficient of metals [16]. The advantage of this model is that it can calculate well for crystals having multiple acoustic phonons with low isotropy and symmetry at both LT and HT regions [17]. Meanwhile, the experimental TE coefficient of Ag was measured by Touloukian et al. [18]. Therefore, the calculation and analysis of the anharmonic TE coefficient of Ag using the ACD model will be a necessary investigation for the thermodynamic parameters of metals.

2. PROBLEM

One usually considers an anharmonic effective (AE) potential [19] to determine the thermodynamic parameters of crystal metals. If ignoring the constant contribution and extending to the third order, this potential is written in the form [20]:

$$V_{eff} = k_{eff} x^2 / 2 - k_{an} x^3, \; x = r - r_0 \tag{1}$$

where k_{eff} is the effective force constant, k_{an} is the anharmonicity force constant, x is the displacement, and r_0 and r are the equilibrium and instantaneous atomic distances, respectively.

The FCC structural model of Ag is illustrated in Fig. 2, which is one of the most stable crystal structures and has the highest packing density [7]. In this structure, each atom has a mass of m and is bonded with other surrounding four atoms [21]. The AE potential [12] can be calculated from the pair interaction potential of atoms, which is written via Morse potential parameters as follows [22]:

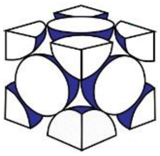

Figure 2. *The FCC structural model of Ag.*

$$V_{eff} = 5D\alpha^2 x^2 / 2 - 5D\alpha^3 x^3 / 4 \tag{2}$$

where D is dissociation energy and $1/\alpha$ is the potential width.

Comparing Eq. (1) with Eq. (2), the local force constants are deduced as follows:

$$k_{eff} = 5D\alpha^2, \quad k_{an} = 5D\alpha^3 / 4 \tag{3}$$

The ACD model [23] is perfected based on the correlated Debye (CD) model [24] and the many-body perturbation (MBP) approach [25] using AE potential that contains correlation effects [19]. In this model, each thermal vibration can be quantized and treated as a phonon that corresponds to a wave having a frequency ω described via the dispersion relation [23]:

$$\omega = \omega_D \left| \sin\left(qa/2 \right) \right|, \; |q| \le \pi/a \tag{4}$$

where a is the lattice constant, and q is the phonon wavenumber in the first Brillouin (FB) zone.

In this model, the correlated Debye frequency ω_D and temperature θ_D of Ag characterize thermal vibrations [16, 17]. They can obtain from the effective force constant k_{eff} as follows:

$$\omega_D = 2\sqrt{k_{eff}/m} = 2\alpha\sqrt{5D/m} \tag{5}$$

$$\theta_D = \frac{\hbar\omega_D}{k_B} = \frac{2\hbar\alpha}{k_B}\sqrt{\frac{5D}{m}} \tag{6}$$

where $\hbar$ is the reduced Planck constant and k_B is the Boltzmann constant.

Normally, the TE coefficient characterizes the net thermal (NT) expansion and can be determined by [26]:

$$\alpha_T = \frac{d\ell}{\ell dT} = \frac{dR}{RdT} = \frac{d\langle r\rangle}{\langle r\rangle dT} \tag{7}$$

where T is the absolute temperature, ℓ is a particular length measurement, R is the atomic distance, and $\langle\ \rangle$ is the thermal average and is approximated via the statistical density matrix.

Usually, the atomic distance $R = \langle r\rangle$ describes the variance of the real radial pair distribution (RPD) function and can be presented via a powerful moment $\langle x\rangle$ of the RPD function [27].

$$R = \langle r_0 + x\rangle = r_0 + \langle x\rangle \quad |q| \le \pi/a \tag{8}$$

Substituting the atomic distance R in Eq. (8) into Eq. (7), the TE coefficient is rewritten as

$$\alpha_T = \frac{d\left(r_0 + \langle x\rangle\right)}{\left(r_0 + \langle x\rangle\right)dT} \simeq \frac{d\left(\langle x\rangle\right)}{r_0 dT} \tag{9}$$

The general temperature-dependent expression of the powerful moment $\langle x\rangle$ in the ACD model was calculated by Hung *et al*. [23]:

$$\langle x\rangle = \frac{3a\hbar k_{an}}{2\pi k_{eff}^2}\int_0^{\pi/a}\omega(q)\frac{1+\exp\left\{\hbar\omega(q)/k_BT\right\}}{1-\exp\left\{\hbar\omega(q)/k_BT\right\}}dq \tag{10}$$

It can be seen this general expression depends on the lattice constant *a*, so it is not optimized yet. To solve this limitation in the ACD model [23], we convert the variable q to the variable $p = qa/2$ and obtain the following expression:

$$\langle x\rangle = \frac{3\hbar k_{an}}{\pi k_{eff}^2}\int_0^{\pi/2}\omega(p)\frac{1+\exp\left\{-\hbar\omega(p)/k_BT\right\}}{1-\exp\left\{-\hbar\omega(p)/k_BT\right\}}dp \tag{11}$$

Substituting the expressions of local force constants k_{eff} and k_{an} of Ag in Eq. (3) into Eq. (10), the temperature-dependent powerful moment $\langle x\rangle$ is written in the form as

$$\begin{aligned}\langle x\rangle &= \frac{3\hbar}{20\pi D\alpha}\int_0^{\pi/2}\omega(p)\frac{1+\exp\left\{-\hbar\omega(p)/k_BT\right\}}{1-\exp\left\{-\hbar\omega(p)/k_BT\right\}}dp\\ &= \frac{3\hbar}{20\pi D\alpha}\int_0^{\pi/2}\omega(p)\coth\left\{\hbar\omega(p)/2k_BT\right\}dp\end{aligned} \tag{12}$$

Using this power moment $\langle x\rangle$ to calculate the temperature-dependent TE *coefficient from Eq. (8)*, we obtain the following result:

$$\alpha_T = \frac{3\hbar}{20\pi D\alpha r_0}d\left\{\int_0^{\pi/2}\omega(p)\coth\left\{\hbar\omega(p)/2k_BT\right\}dp\right\}\Big/dT \tag{13}$$

Approximating an expression $\exp\left\{-n\hbar\omega(p)/k_BT\right\} \approx 0$ with $n > 1$, we calculate the TE *coefficient* of Ag in the LT limit ($T \to 0$) from Eq. (12). The obtained result is

$$\alpha_T \simeq \pi k_B^2 T/10\hbar r_0\omega_D D\alpha \tag{14}$$

Approximating an expression $\exp\left\{\hbar\omega(p)/k_BT\right\} \approx 1 + \hbar\omega(p)/k_BT$, we calculate the TE *coefficient* of Ag in the HT limit ($T \to \infty$) from Eq. (12). The obtained results are:

$$\alpha_T \simeq 3k_B/20r_0D\alpha \tag{15}$$

Thus, the ACD model has been extended to efficiently calculate the anharmonic TE coefficient of Ag. The obtained expression has been more optimized than the previous ACD model. This expression also can satisfy all their temperature-dependent fundamental properties.

3. RESULTS AND DISCUSSION

In *numerical* calculations of Ag, we use the atomic mass $m = 107{,}868\,\text{u}$ [28] and Morse potential parameters $r_0 = 2.877$ Å, $\alpha = 2.062$ Å^{-1}, and $D = 0.121\,\text{eV}$ were determined from the experimental XAFS data using the method proposed by I.V. Pirog for metal crystals [29]. From these obtained comparisons, we analyze and discuss the efficacy of the ACD model in investigating the anharmonic TE coefficient of Ag.

Use of Eqs. (3)-(6), we calculate the thermodynamic parameters of Ag and obtain the local force constants $k_{eff} = 2.572\,\text{eVÅ}^{-2}$ and $k_{an} = 1.326\,\text{eVÅ}^{-3}$, the correlated Debye frequency $\omega_D = 3.034 \times 10^{13}\,\text{Hz}$, and the correlated Debye temperature $\theta_D \simeq 231.737\,\text{K}$. Meanwhile, the determined corresponding values from the experimental Morse potential parameters $D = 0.3323\,eV$ and $\alpha = 1.3190\,\AA^{-1}$ by Girifalco & Weizer [22], which are $k_{eff} = 2.891\,\text{eVÅ}^{-2}$, $k_{an} = 0.953\,\text{eVÅ}^{-3}$, $\omega_D = 3.216 \times 10^{13}\,\text{Hz}$, and $\theta_D \simeq 245.654\,\text{K}$. And the determined corresponding values from the experimental local force constants by Newville & Stern [29], which are $k_{eff} = 2.959\,\text{eVÅ}^{-2}$, $k_{an} = 1.298\,\text{eVÅ}^{-3}$, $\omega_D = 3.254 \times 10^{13}\,\text{Hz}$, and $\theta_D \simeq 245.654\,\text{K}$. It can be seen that our results are suitable with the obtained values from experiments [25], especially for the correlated Debye temperature and frequency.

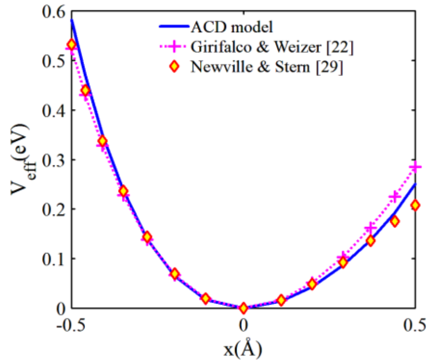

Figure 3. *The position-dependent AE potential of Ag is obtained using the present model and experimental data.*

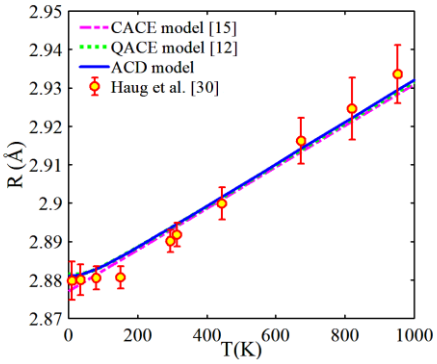

Figure 4. *The temperature-dependent atomic distance of Ag is obtained using the theoretical models and experimental data.*

The position-dependence AE potential $V_{eff}(x)$ of Ag in the position range from $x = -0.5$ Å to $x = 0.5$ Å is represented in Fig. 3. Our obtained result using the ACD model is calculated by Eq. (2), and other values are obtained from Eq. (1) with the experimental data of the local force constants determined by Girifalco & Weizer [22] and Newville & Stern [29]. The obtained results show that the graph representing the AE potential is asymmetric, in which the values at the positive positions are smaller than those at the negative positions of the same magnitude. This property is due to the contribution of the anharmonic component $\left(-k_{an}x^3\right)$ to the AE potential, especially at positions far from the equilibrium position ($x = 0$) with large thermal vibrations at high temperatures.

The temperature-dependent atomic distance $R(T)$ of Ag in a range from 0 to 1000 K is represented in Fig. 4. Our obtained result using the present ACD model is calculated by Eqs. (8)

and (12), and the obtained result using the CACE [15] and QACE [12] models are calculated by Eq. (8) with the temperature-dependent power moment $\langle x \rangle$ from Refs. [15] and [12]. Meanwhile, the experimental data at 10 K, 35 K, 80 K, 150 K, 294 K, 313 K, 443 K, 673 K, 820 K, and 952 K are measured by Haug et al. at the HASYLAB (DESY, Hamburg, Germany) [30]. It can be seen that our result agrees well with those obtained using the CACE (exclusion for the LT region) [15] and QACE [12] models and experimental data [30]. For example, the obtained results using the ACD model, CACE model, QACE model, and experimental data at $T = 294\ K$ are $R \simeq 2.9031$, $R \simeq 2.9009\,\text{Å}$ [15], $R \simeq 2.9014\,\text{Å}$ [12], and $R \simeq 2.8987\,\text{Å}$ [30], respectively. Moreover, the CACE model cannot calculate quantum effects using classical statistical theory [15], so this model cannot work well in the LT region, and the obtained result approaches zero as the temperature approaches zero.

The temperature-dependent TE *coefficient* $\alpha_T(T)$ of Ag in a range from 0 to 1000 K is represented in Fig. 5. Our obtained result using the present ACD model is calculated by Eq. (13), and the experimental values are determined by Touloukian et al. [18]. Meanwhile, the obtained results using the CACE [15] and QACE [12] models are calculated by Eq. (9) with the temperature-dependent power moment $\langle x \rangle$ determined from Refs. [15] and [12].

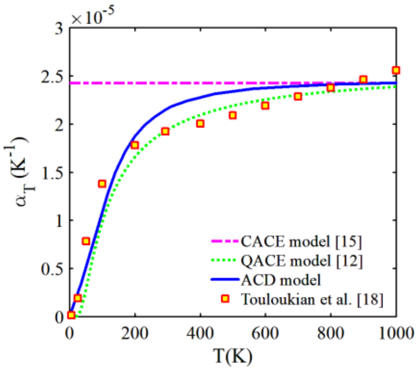

Figure 5. *The temperature-dependent TE coefficient of Ag is obtained using the theoretical models and experimental data.*

It can be seen that our result increases rapidly with increasing temperature *T* and approaches those obtained using the CACE model [15] in the HT limit, which fits perfectly with Eq. (13) and shows that the present ACD model can efficiently describe the anharmonic effects. The obtained result using the CACE model [15] is constant and is not satisfied with the experimental values in the LT region. It is because the temperature-dependent atomic distance is a linear function, and the quantum effects are not considered in this model.

Table 1. *The TE coefficient of Ag is obtained using the theoretical models and experimental data.*

Quantity	Value												
T (K)	5	25	50	100	200	293	400	500	600	700	800	900	1000
α ($\times10^{-5}$ K^{-1})^a	0.02	0.24	0.50	1.09	1.86	2.13	2.26	2.32	2.35	2.37	2.39	2.40	2.40
α ($\times10^{-5}$ K^{-1})^b	0.00	0.02	0.28	0.98	1.66	1.93	2.09	2.19	2.25	2.30	2.33	2.36	2.39
α ($\times10^{-5}$ K^{-1})^c	0.00	0.19	0.82	1.42	1.78	1.89	1.97	2.06	2.15	2.26	2.37	2.48	2.59

[a] *Our values are obtained using the present ACD model.*

[b] *The values are obtained using the QACE model determined from Ref. [12].*

[c] *The values are obtained from the experimental data determined by Touloukian et al. [18].*

The obtained values of the TE *coefficient* using different methods are given in Table 1. It can be seen that our values agree with those obtained from the QACE model [12] and experimental data [18], especially in the HT region. Moreover, in the LT region, the obtained values using the QACE model [12] are smaller than those obtained using the present ACD model. It is because both these models take into account the quantum effects, but the QACE [12] uses only one effective frequency without considering the frequency dispersion as in the present ACD model.

4. CONCLUSIONS

In this investigation, we have performed an efficient ACD model in analyzing and calculating the anharmonic TE coefficient of Ag. The calculated temperature-dependent TE coefficient using the present ACD model can satisfy all its fundamental properties. This ACD model has used the AE potential, so this model contains the correlation effects between atoms in the many-body perturbation approach.

The rapid increase of the TE coefficient with increasing temperature T shows that the lattice expands more strongly at high temperatures. This result can indicate the influence of anharmonic effects in the HT region and the influence of quantum effects in the LT region on the anharmonic TE coefficient.

The good agreement of our results of Ag with those obtained using the QACE model and experimental data at various temperatures demonstrates the efficacy of the ACD model in investigating the anharmonic TE coefficient. The present ACD model can be used to calculate and analyze the anharmonic TE coefficient of other metals in both the LT and HT regions.

Acknowledgment: *This investigation was supported by the University of Fire Prevention and Fighting, 243 Khuat Duy Tien, Thanh Xuan, Hanoi, Vietnam.*

REFERENCES

[1]. H. Liu, W. Sun, Z. Zhang, L. Lovings, and C. Lind, *"Thermal Expansion Behavior in the $A_2M_3O_{12}$ Family of Materials,"* Solids, vol. 2, no. 1, pp. 87-107, (2021).

[2]. J. W. Hwang, *"Thermal expansion of nickel and iron, and the influence of nitrogen on the lattice parameter of iron at the Curie temperature,"* Masters Theses, Missouri: University of Missouri-Rolla, (1972).

[3]. V. A. Drebushchak, *"Thermal Expansion of Solids: Review on Theories,"* Journal of Thermal Analysis and Calorimetry, vol. 142, pp. 1097-1113, (2020).

[4]. G. Laplanche, P. Gadaud, O. Horst, F. Otto, G. Eggeler, and E. P. George, *"Temperature Dependencies of the Elastic Moduli and Thermal Expansion Coefficient of an Equiatomic, Single-Phase CoCrFeMnNi High-Entropy Alloy,"* Journal of Alloys and Compounds, vol. 623, pp. 348-353, (2015).

[5]. P. Eisenberger and G. S. Brown, *"The study of disordered systems by EXAFS: Limitations,"* Solid State Communications, vol. 29, no. 6, pp. 481-484, (1979).

[6]. Z. K. Liu, Y. Wang, and S. Shang, *"Thermal Expansion Anomaly Regulated by Entropy,"* Scientific Reports, vol. 4, p. 7043, (2014).

[7]. J. Emsley, *"Nature's Building Blocks: An A-Z Guide to the Elements,"* 2nd edition, New York: Oxford University Press, (2011).

[8]. C. R. Hammond, *"The Elements, in Handbook of Chemistry and Physics,"* 81st edition, Boca Raton: CRC Press, (2004).

[9]. J. Y. *Maillard and P. Hartemann, "Silver as an antimicrobial: Facts and gaps in knowledge,"* Critical Reviews in Microbiology, vol. 39, no. 4, pp. 373-83, (2012).

[10]. N. V. Hung, C. S. Thang, N. B. Duc, D. Q. Vuong, and T. S. Tien, *"Temperature Dependence of Theoretical and Experimental Debye-Waller Factors, Thermal Expansion and XAFS of Metallic Zinc,"* Physica B: Condensed Matter, vol. 521, pp. 198-203, (2017).

[11]. N. V. Hung, C. S. Thang, N. B. Duc, D. Q. Vuong, and T. S. Tien, *"Advances in theoretical and experimental XAFS studies of thermodynamic properties, anharmonic effects and structural determination of fcc crystals,"* European Physical Journal B, vol. 90, p. 256, (2017).

[12]. T. S. Tien, *"Advances in Studies of the Temperature Dependence of the EXAFS Amplitude and Phase of FCC Crystals,"* Journal of Physics D: Applied Physics, vol. 53, no. 11, p. 315303, (2020).

[13]. T. S. Tien, *"Investigation of the anharmonic EXAFS oscillation of distorted HCP crystals based on*

extending quantum anharmonic correlated Einstein model," Japanese Journal of Applied Physics, vol. 60, no. 11, p. 112001, (2021).

[14]. N. V. Hung, T. S. Tien, N. B. Duc, and D. Q. Vuong, *"High-order expanded XAFS Debye-Waller factors of HCP crystals based on classical anharmonic correlated Einstein model,"* Modern Physics Letters B, vol. 28. no. 21, p. 1450174, (2014).

[15]. T. S. Tien, *"Analysis of EXAFS oscillation of FCC crystals using classical anharmonic correlated Einstein model,"* Radiation Physics and Chemistry, vol. 186, p. 109504, (2021).

[16]. T. S. Tien, N. T. M. Thuy, V. T. K. Lien, N. T. N. Anh, D. N. Bich, and L. Q. Thanh, *"Calculation of Temperature-Dependent Thermal Expansion Coefficient of Metal Crystals Based on Using Anharmonic Correlated Debye Model,"* Advances in Technology Innovation, vol. 8, no. 1, pp. 73-80, (2023).

[17]. T. S. Tien, *"Analysis of EXAFS oscillation of monocrystalline diamond-semiconductors using anharmonic correlated Debye model,"* European Physical Journal Plus, vol. 136, p. 539, (2021).

[18]. Y. S. Touloukian, R. K. Kirby, R. E. Taylor, and P. D. Desai, *"Thermophysical Properties of Matter,"* New York: Plenum, vol. 12, p. 298, (1975).

[19]. N. V. Hung and J. J. Rehr, *"Anharmonic correlated Einstein-model Debye-Waller factors,"* Physical Review B, vol. 56, no. 1, pp. 43-46, (1997).

[20]. A. I. Frenkel and J. J. Rehr, *"Thermal expansion and x-ray-absorption fine-structure cumulants,"* Physical Review B, vol. 48, no. 1, pp. 585-588, (1993).

[21]. S. H. Simon, *"The Oxford Solid State Basics,"* 1st *edition, Oxford: Oxford* University Press, (2013).

[22]. L. A. Girifalco and V. G. Weizer, *"Application of the Morse Potential Function to Cubic Metals,"* Physical Review, vol. 114, no. 3, pp. 687-690, (1959).

[23]. N. V. Hung, N. B. Trung, and B. Kirchner, *"Anharmonic correlated Debye model Debye-Waller factors,"* Physica B: Condensed Matter, vol. 405, pp. 2519-2525, (2010).

[24]. G. Beni and P. M. Platzman, *"Temperature and polarization dependence of extended x-ray absorption fine-structure spectra,"* Physical Review B, vol. 14, no. 4. pp. 1514-1518, (1976).

[25]. G. D. Mahan, *"Many-Particle Physics,"* 2nd edition, New York: Plenum, (1990).

[26]. C. Y. Ho, R. E. Taylor, *"Thermal Expansion of Solids,"* Materials Park: ASM International, (1998).

[27]. L. Tröger, T. Yokoyama, D. Arvanitis, T. Lederer, M. Tischer, and K. Baberschke, *"Determination of bond lengths, atomic mean-square relative displacements, and local thermal expansion by means of soft-x-ray photoabsorption,"* Physical Review B, vo. 49, no. 2, pp. 888-903, (1994).

[28]. N. W. Ashcroft and N. D. Mermin, *"Solid State Physics,"* 1st edition, New York: Holt-Rinehart & Winston, (1976).

[29]. I. V. Pirog, T. I. Nedoseikina, I. A. Zarubin, A. T. Shuvaev, *"Anharmonic pair potential study in face-centered-cubic structure metals,"* Journal of Physics: Condensed Matter, vol. 14, pp. 1825-1832, (2002).

[30]. J. Haug, A. Chassé, R. Schneider, H. Kruth, and M. Dubiel, *"Thermal expansion and interatomic potentials of silver revealed by extended x-ray absorption fine structure spectroscopy using high-order perturbation theory,"* Physical Review B, vol. 77, p. 184115, (2008).

TÓM TẮT

Phân tích hệ số giãn nở nhiệt phi điều hòa của tinh thể bạc

Hệ số giãn nở nhiệt phi điều hòa (TE) của tinh thể bạc (Ag) đã được tính toán và phân tích trong sự phụ thuộc vào nhiệt độ. Mô hình tính toán được phát triển dựa trên mô hình Debye tương quan và phương pháp nhiễu loạn nhiều hạt bằng cách sử dụng hàm thế hiệu dụng phi điều hòa. Các tham số nhiệt động của mạng tinh thể bắt nguồn từ ảnh hưởng của các dao động nhiệt của tất cả các nguyên tử. Tính phi điều hòa được xem như là kết quả của các tương tác phonon-phonon với mỗi dao động nguyên tử có thể được lượng tử hóa và coi như là một phonon. Biểu thức thu được của hệ số TE phi điều hòa của Ag có thể thỏa mãn tất cả các tính chất cơ bản phụ thuộc vào nhiệt độ của chúng. Kết quả tính số của Ag phù hợp tốt với các kết quả thu được từ các mô hình lý thuyết khác và dữ liệu thực thực nghiệm ở các nhiệt độ khác nhau trong phạm vi từ 0 K đến 1000 K. Kết quả thu được cho thấy mô hình hiện tại hiệu quả trong việc nghiên cứu hệ số TE phi điều hòa của Ag.

Từ khóa: Hệ số dãn nở nhiệt phi điều hòa; Tinh thể bạc; Mô hình Debye tương quan phi điều hòa.