

**DETERMINE MORSE POTENTIAL, THERMAL EXPANSION COEFFICIENT AND
DESCRIBE ASYMMETRICAL COMPONENTS THROUGH DEBYE -WALLER FACTOR
BY ANHARMONIC CORRELATED EINSTEIN MODEL**

Xác định thế Morse, hệ số dẫn nở nhiệt và mô tả các thành phần bất đối xứng qua hệ số Debye - Waller bằng mô hình Einstein tương quan phi điều hòa

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TÓM TẮT

Thế tương tác hiệu dụng trong mô hình Einstein tương quan phi điều hòa đã được xây dựng dựa trên cơ sở tính giải tích thế tương tác Morse giữa cặp nguyên tử hấp thụ và tán xạ với các nguyên tử lân cận gần nhất, nghiên cứu đã biểu diễn hệ thức hệ số dẫn nở nhiệt tại nhiệt độ cao và các biểu thức mô tả thành phần bất đối xứng (cumulant) và các đại lượng nhiệt động qua hệ số Debye-Waller. Hệ thức hàm tương quan giữa các cumulant, hàm tương quan giữa các cumulant và hệ số dẫn nở nhiệt đối với các tinh thể có cấu trúc lập phương cũng đã được xác định. Các hệ thức nhận được bao chứa cả lý thuyết cổ điển tại nhiệt độ cao và hiệu ứng lượng tử tại nhiệt độ thấp.

Từ khóa: *Phi điều hòa; tương quan; nhiệt động; bất đối xứng; cumulant.*

ABSTRACT

Effective potential in anharmonic correlated Einstein model was determined on to base analytics calculation Morse potential between absorber and backscatter atoms with nearest neighbor atoms, this work was represented the expression of thermal expansion coefficient at high temperatures and expressions was described ansymmetry components (cumulants) and thermodynamic quantity through Debye-Waller factor. Expressions of correlative function between the cumulants and between cumulants and thermal expansion coefficient for cubic structural crystals also was determined. The expressions obtained include classical theory at high temperature and quantum effects at low temperature.

Keyword: *Anharmonic; correlate; thermodynamic; ansymmetry; cumulant.*

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1. Introduction

Anharmonic correlated Einstein model was used the calculation cumulants, frequency and temperature Einstein and thermodynamic parameters of the cubic structural crystals, results obtained agree well with experimental values [6]. In the Einstein model, atomic interaction potential is Morse pairs potential, however Morse potential usually deduced from experiment [4], so analytics calculation the physics quantity when to need Morse potential be very hard, therefore if thermodynamic parameters of Morse potential are calculated in advance will reduce the number calculations. In this studying scope, we are will analytics calculation in advance Morse interactive potential in anharmonic correlated Einstein model and application to determine the expressions of thermal expansion coefficient, build the expressions thermodynamic parameters and cumulants through Debye-Waller factor, consider correlative functions and thermodynamics parameters in classical approximation at high temperature and quantum effects at low temperature.

2. Formalism

Anharmonic correlated Einstein model is described by effective interaction potential as form [1, 9]:

$$U_E(x) \approx \frac{1}{2}k_{\text{eff}}x^2 + k_3x^3 + \dots \quad (1)$$

In which $x = r - r_0$ is deviation of the instantaneous bond length of two atoms from their equilibrium distance or the location of the minimum potential interaction, k_{eff} is effective spring constant, because it include all contributions of neighbor atoms, k_3 is anharmonicity parameter and describing an asymmetry in interactive potential.

Anharmonic correlated Einstein model is determined by vibration of single pairs atoms with M_1 and M_2 mass of absorber and backscatter atoms. Vibration of atoms affected by neighbor atoms so interactive potential in expression (1) is written as form [6]:

$$U_E(x) = U(x) + \sum_{j \neq i} U\left(\frac{\mu}{M_i}x\hat{\mathbf{R}}_{oi}\hat{\mathbf{R}}_{ij}\right) \quad (2)$$

with $\mu = \frac{M_1M_2}{M_1 + M_2}$ is reduced mass, $\hat{\mathbf{R}}$ is the unit bond length vector, $U(x)$ characterize to the single pairs potential between absorber and backscatter atoms, the second term in equation (2) characterize for contribution of nearest neighbors atoms and calculation by sum i which is over absorber ($i=1$) and backscatter ($i=2$), and the sum j which is over all their nearest neighbors, excludes the absorber and backscatter themselves because they contribute in the $U(x)$.

The atomic vibration is calculated on based quantum statistical procedure with approximate quasi - harmonic vibration [1], in which the Hamiltonian of the system is written as harmonic term with respect to the equilibrium at a given temperature plus an anharmonic perturbation. Taking account from that we have:

$$\begin{aligned} H &= \frac{P^2}{2\mu} + U_E(x) = \frac{P^2}{2\mu} + \frac{1}{2}k_{\text{eff}}x^2 + k_3x^3 + \dots = \\ &= \frac{P^2}{2\mu} + \frac{1}{2}k_{\text{eff}}(y+a)^2 + k_3(y+a)^3 + \dots \\ &= \frac{P^2}{2\mu} + \frac{1}{2}k_{\text{eff}}(y^2 + 2ay + a^2) + k_3(y^3 + a^3 + 3a^2y + 3ay^2) + \dots = \\ &= \frac{P^2}{2\mu} + \left(\frac{1}{2}k_{\text{eff}}a^2 + k_3a^3 \right) + \\ &+ y\left(k_{\text{eff}}a + 3k_3a^2\right) + y^2\left(\frac{1}{2}k_{\text{eff}} + 3k_3a\right) + k_3y^3 + \dots \quad (3) \end{aligned}$$

Setup H_0 is sum of first term and fourth term, $U_E(a)$ is second term and $\delta U_E(y)$ is sum of

third term and fifth term, we have expressions:

$$H_0 = \frac{P^2}{2\mu} + \frac{k}{2} y^2, \quad \frac{k}{2} = \frac{k_{eff}}{2} + 3k_3 a \quad (4)$$

$$U_E(a) = \frac{1}{2} k_{eff} a^2 + k_3 a^3 \quad (5)$$

$$\delta U_E(a) = (k_{eff} a + 3k_3 a^2) y + k_3 y^3 \quad (6)$$

Expression (3) will become:

$$H = H_0 + U_E(a) + \delta U_E(y) \quad (7)$$

in which a is thermal expansion coefficient with:

$$x = r - r_0, \quad y = x - a,$$

$$a = \langle x \rangle \rightarrow \langle y \rangle = \langle x - a \rangle = \langle r - r_0 - r + r_0 \rangle = 0$$

From equation (7) deduced interactive potential according to anharmonic correlated Einstein model can write as form:

$$U_E(x) = U_E(a) + \frac{1}{2} k_{eff} y^2 + \delta U_E(y) \quad (8)$$

In anharmonic correlated Einstein model, interactive potential is Morse pairs anharmonic potential [5], consider approximation for cubic structural crystals, Morse anharmonic potential as form: $U(r) = D(e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)})$ (9)

in which $\alpha(\text{\AA}^{-1})$ is thermal expansion coefficient, $D(\text{eV})$ is the dissociation energy by $U(r_0) = -D$.

We can write expression of Morse potential according to form of x :

$$U(r) = D(e^{-2\alpha x} - 2e^{-\alpha x}) \quad (10)$$

Expand the equation (10) according to x , we have:

$$U(x) = D \left[1 + \frac{-2\alpha x}{1!} + \frac{(-2\alpha x)^2}{2!} + \frac{(-2\alpha x)^3}{3!} + \frac{(-2\alpha x)^4}{4!} + \dots \right]$$

$$\left. - 2 \left(1 + \frac{(-\alpha x)}{1!} + \frac{(-\alpha x)^2}{2!} + \frac{(-\alpha x)^3}{3!} + \frac{(-\alpha x)^4}{4!} + \dots \right) \right] = D \left[1 - 2\alpha x + 2\alpha^2 x^2 - \frac{4}{3} \alpha^3 x^3 + \frac{2}{3} \alpha^4 x^4 + \dots - 2 \left(1 - \alpha x + \frac{1}{2} \alpha^2 x^2 - \frac{1}{6} \alpha^3 x^3 + \frac{1}{12} \alpha^4 x^4 \right) \right]$$

Taking approximate to the third-order term, we can write reduction:

$$U(x) \approx D \left[1 - 2\alpha x + 2\alpha^2 x^2 - \frac{4}{3} \alpha^3 x^3 - 2 + 2\alpha x - \alpha^2 x^2 + \frac{1}{3} \alpha^3 x^3 + \dots \right]$$

Thus, expression of Morse potential according to deviation of the instantaneous bond length of two atoms x will write become:

$$U(x) = D(-1 + \alpha^2 x^2 - \alpha^3 x^3 + \dots) \quad (11)$$

The interaction between pairs atoms in anharmonic correlated Einstein model is described by expression effective interaction potential of Morse pairs anharmonic potential in eq. (11).

From equations (2) and (11) we have:

$$U_E(x) = D(-1 + \alpha^2 x^2 - \alpha^3 x^3 + \dots) + \sum_{j \neq i} U \left(\frac{\mu}{M_i} x \hat{R}_{0i} \hat{R}_{ij} \right) \quad (12)$$

With cubic structural crystals and pure, mass of absorber and backscatter atoms is equal, so can take approximation $M_1 \approx M_2 \approx M \rightarrow \mu = \frac{M}{2}$, simultaneously expand second term of eq.(12) and calculation, we deduced thermodynamic parameters $k_3, k_{eff}, \delta U(E)$ [1, 10].

$$k_{eff} = c_3(D\alpha^2 + c_2 a k_3) = \mu \omega_E^2, \quad k_3 = -c_1 D \alpha^3 \quad (13)$$

$$\delta U_E(y) = D \alpha^2 (c_3 a y - c_1 \alpha y^3) \quad (14)$$

in which c_1, c_2, c_3 are structural parameters with values corresponding has determined [5].

Anharmonic correlated Einstein model have been used to analytics calculation cumulants [6], the expand cumulants according to the expression:

$$e^{(2i k r)} = \exp \left[2i k r_0 + \sum_n \frac{(2i)^n}{n!} \sigma^{(n)} \right]; n=1,2,3.. \quad (15)$$

with $\sigma^{(n)}$ are cumulants and $x = r - r_0$ is

thermal expansion coefficient and $a(T) = \langle r - r_0 \rangle = \sigma^{(1)}$; $y = x - a$, $\langle y \rangle = 0$.

Expand cumulants from the first-order to the sixth-order, we have:

$$\begin{aligned} \sigma^{(1)} &= R - r; \langle y \rangle = 0 \\ \sigma^{(2)} &= \sigma^2 = \langle (r-R)^2 \rangle = \langle y^2 \rangle; \\ \sigma^{(3)} &= \langle (r-R)^3 \rangle = \langle y^3 \rangle; \\ \sigma^{(4)} &= \langle (r-R)^4 \rangle - 3\langle (r-R)^2 \rangle^2 = \langle y^4 \rangle - 3\langle \sigma^2 \rangle^2 \\ \sigma^{(5)} &= \langle (r-R)^5 \rangle - 10\langle (r-R)^3 \rangle \langle (r-R)^2 \rangle = \langle y^5 \rangle - 10\langle y^3 \rangle \langle \sigma^2 \rangle; \\ \sigma^{(6)} &= \langle (r-R)^6 \rangle - 15\langle (r-R)^4 \rangle \langle (r-R)^2 \rangle - 10\langle (r-R)^3 \rangle^2 + 30\langle (r-R)^2 \rangle^3 \\ &= \langle y^6 \rangle - 15\langle y^4 \rangle \langle \sigma^2 \rangle - 10\langle y^3 \rangle^2 + 30\langle \sigma^2 \rangle^3. \end{aligned} \quad (16)$$

In above expressions of cumulants, the second cumulant $\sigma^{(2)} = \sigma^2$ or the mean square relative displacement (MSRD) otherwise known as Debye-Waller factor (DWF).

Expressions analytics calculation cumulants for cubic structure crystals has determined from the first-order to the third-order cumulants [10, 5], as form:

The first cumulant or net expansion coefficient

$$\sigma^{(1)} = a = \frac{3c_3 \hbar \omega_E (1+z)}{2c_1^2 D \alpha (1-z)} \quad (17)$$

The second cumulant or Debye-Waller factor:

$$\sigma^{(2)} = \langle y^2 \rangle = \frac{\hbar \omega_E (1+z)}{2c_1 D \alpha^2 (1-z)} \quad (18)$$

The third cumulant characterize to the anharmonicity:

$$\sigma^{(3)} = \frac{3c_3 (\hbar \omega_E)^2 (1+10z+z^2)}{2D^2 \alpha^3 c_1^3 (1-z)^2} \quad (19)$$

Next, we calculate thermal expansion coefficient due to effect of anharmonicity when high raise temperature by fomula [1, 3]:

$$\alpha_T = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P$$

(20)

in which V is volume corresponding the change of absolute temperature T under pressure P. Use equation state of thermal system:

$$\begin{aligned} \left(\frac{\partial P}{\partial T} \right)_V \left(\frac{\partial T}{\partial V} \right)_P \left(\frac{\partial V}{\partial P} \right)_T &= -1 \\ \Rightarrow \left(\frac{\partial T}{\partial V} \right)_P &= - \frac{1}{\left(\frac{\partial P}{\partial T} \right)_V \left(\frac{\partial V}{\partial P} \right)_T} \end{aligned} \quad (21)$$

From expressions (20) and (21), we have:

$$\alpha_T = \frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T \left(\frac{\partial P}{\partial T} \right)_V \quad (22)$$

Setup $K = -V \left(\frac{\partial P}{\partial V} \right)_T$ is elastic modulus

determination the change of volume due to interaction of pressure. Ignore links between vibrations of atoms and assume freedom energy Helmholtz as form $F = U + \sum_q F_q$ with U

is sum potential energy, F_q is free energy and was created from vibration of lattice with wave vector q, then pressure dependence to volume according to expression [2,5]:

$$P = - \left(\frac{\partial F}{\partial V} \right)_T = - \frac{dU}{dV} - \sum_q \frac{dF_q}{dV} = - \frac{dU}{dV} - \sum_q \hbar \frac{\partial \omega_q}{\partial V} \left[\frac{1}{2} + \frac{1}{\exp\left(\frac{\hbar \omega_q}{k_B T} - 1\right)} \right] \quad (23)$$

When appearance anharmonic effect, the system equilibrium at new location and volume expanded so important phenomena of anharmonic effect is dependence of frequency net vibration to volume, this dependence described through by second term in expression (23).

To simple, assume dependence to volume of all frequencies net vibration the same and write through Gruneisen factor as

form:

$$\omega \sim V^{-\gamma_G} \Rightarrow \gamma_G = -\frac{\partial(\ln\omega)}{\partial(\ln V)} = -\frac{\partial(\ln\omega)}{\partial a} \frac{\partial a}{\partial r} \frac{\partial r}{\partial(\ln V)} \quad (24)$$

Factor γ_G characterize for anharmonic effect with net thermal coefficient:

$$a = r - r_0 \rightarrow \frac{\partial a}{\partial r} = 1$$

Simultaneously we have:

$$a(T) - a(T_0) = da = \alpha_T r dT$$

Deduce thermal expansion coefficient: $\alpha_T = \frac{1}{r} \frac{da}{dT}$ (25)

Substitute (17) into (25) we get:

$$\begin{aligned} \alpha_T &= \frac{3c_3 \hbar \omega_E}{2c_1^2 D\alpha r} \frac{d}{dT} \left(\frac{1+z}{1-z} \right) = \frac{3c_3 \hbar \omega_E}{2c_1^2 D\alpha r} \frac{d}{dT} \left(\frac{1+e^{-\theta_E/T}}{1-e^{-\theta_E/T}} \right) = \\ &= \frac{3c_3 \hbar \omega_E}{2c_1^2 D\alpha r} \frac{(1-e^{-\theta_E/T})e^{-\theta_E/T} \frac{\theta_E}{T^2} - (1-e^{-\theta_E/T})(-e^{-\theta_E/T}) \frac{\theta_E}{T^2}}{(1-e^{-\theta_E/T})^2} = \\ &= \frac{3c_3 \hbar \omega_E}{2c_1^2 D\alpha r} \frac{(1-z)z \frac{\theta_E}{T^2} + (1+z)z \frac{\theta_E}{T^2}}{(1-z)^2} = \frac{3c_3 \hbar \omega_E}{2c_1^2 D\alpha r} \frac{2z \frac{\theta_E}{T^2}}{(1-z)^2} = \\ \Rightarrow \alpha_T &= \frac{3c_3 \hbar \omega_E}{c_1^2 D\alpha r} \frac{\theta_E}{T^2} \frac{z}{(1-z)^2} \end{aligned}$$

with $\theta_E = \frac{\hbar \omega}{k_B}$ we have:

$$\alpha_T = \frac{3c_3}{c_1^2 D\alpha r} \frac{(\hbar \omega_E)^2}{k_B T^2} \frac{z}{(1-z)^2} = \frac{3c_3 k_B}{c_1^2 D\alpha r} \left(\frac{\hbar \omega_E}{k_B T} \right)^2 \frac{z}{(1-z)^2};$$

replace $\frac{\hbar \omega_E}{k_B T} = \ln z$, we obtained thermal expansion coefficient:

$$\alpha_T = \frac{3c_3 k_B}{c_1^2 D\alpha r} \frac{z(\ln z)^2}{(1-z)^2}. \quad (26)$$

To reduce calculated and measure, to need simplification the description expressions of thermodynamic parameters, thus we can description thermodynamic parameters through DWF σ^2 [6,7,8] by:

$$z = \frac{\sigma^2 - \sigma_0^2}{\sigma^2 + \sigma_0^2} \quad (27)$$

Substitute formula (27) into equations (17, 18, 19, 26), we have:

$$\sigma^{(1)} = \sigma_0^{(1)} \frac{1+z}{1-z} = \frac{3c_3 \alpha}{c_1} \sigma^2; \quad \sigma_0^{(1)} = \frac{3c_3 \alpha}{c_1} \sigma_0^2 \quad (28)$$

$$\sigma^2 = \sigma_0^2 \frac{1+z}{1-z}; \quad \sigma_0^2 = \frac{\hbar \omega_E}{2c_1 D\alpha r^2} \quad (29)$$

$$\sigma^{(3)} = \sigma_0^{(3)} \frac{3(\sigma^2)^2 - 2(\sigma_0^2)^2}{(\sigma_0^2)^2}; \quad \sigma_0^{(3)} = \frac{3c_3 \alpha}{c_1} (\sigma_0^2)^2 \quad (30)$$

$$\alpha_T = \alpha_T^0 \left(\frac{c_1 D\alpha^2 \sigma^2}{k_B T} \right)^2 \left[1 - \left(\frac{\sigma_0^2}{\sigma^2} \right)^2 \right]; \quad \alpha_T^0 = \frac{3c_3 k_B}{c_1^2 D\alpha r} \quad (31)$$

Simultaneously we deduce correlative expressions between cumulants together and between cumulants with thermal expansion coefficient α_T , distance between atoms r and absolute temperature T according to structural parameters and Debye-Waller factor:

$$\frac{\alpha_T r T \sigma^2}{\sigma^{(3)}} = \frac{c_1 D\alpha^2 \sigma^2}{2k_B T} \frac{1 - \left(\frac{\sigma_0^2}{\sigma^2} \right)^2}{1 - \frac{2}{3} \left(\frac{\sigma_0^2}{\sigma^2} \right)^2};$$

$$(32) \frac{\sigma^{(1)} \sigma^2}{\sigma^{(3)}} = \frac{1}{2 - \frac{4}{3} \left(\frac{\sigma_0^2}{\sigma^2} \right)^2}$$

(33)

where $\sigma_0^{(1)}, \sigma_0^2$ and $\sigma_0^{(3)}$ are contributions zero-point into $\sigma^{(1)}, \sigma^2$ and $\sigma^{(3)}$, structural parameters was described in [5].

According to the description above, outside the Morse potential parameters analytics calculation, to calculate cumulants $\sigma^{(1)}, \sigma^2, \sigma^{(3)}$ and thermal expansion coefficient α_T , we only need to calculate DWF σ^2 , therefore has reduce analytics calculation and programmable calculator for thermodynamic parameters. The expressions is determined from quantum theory, therefore

can applying for any temperature, at high temperature it include approximate results of classical theory and at low temperature limit it always shows quantum effects through contributions of zero-point energy.

In high temperature limit (HT) we use approximate formula $e^x \approx 1 + x$, and approximate change $z = e^{-\frac{\theta_E}{T}}$ with $\theta_E = \frac{\hbar\omega_E}{k_B}$, deduced:

$$z \approx 1 - \frac{\hbar\omega_E}{k_B T} \quad (34)$$

$$\text{We get: } \frac{1+z}{1-z} \approx \frac{2 - \frac{\hbar\omega}{k_B T}}{\frac{\hbar\omega}{k_B T}} = \frac{2k_B T - \hbar\omega}{\hbar\omega} \quad (35)$$

so we reduce expressions of cumulants and thermodynamic parameters at high temperature (see in Table statistic)

In low temperature limit (LT) we use approximate formulas:

$$\frac{1}{1-z} \approx 1+z; \frac{1+z}{1-z} \approx 1+z+z=1+2z \quad (36)$$

because in low temperature limit $z \rightarrow 0$, thus, we can ignore z^2 and higher powers, we reduce expressions of cumulants and thermodynamic parameters at low temperature limit (see in Table statistic).

Note cumulants $\sigma^{(1)}$, σ^2 , $\sigma^{(3)}$ include contributions zero-point energy, α_T approaching the value constant α_T^0 at high temperatures but they destructively according to exponential of $\frac{\theta_E}{T}$ at low temperature and both correlative expressions (32) and (33) approximately with classical results and experiment as 1/2 at high temperatures and right reflection with results of classical theory and experimentalist.

Table 1: Expressions of cumulants, thermal expansion coefficient, correlative expressions at low temperature limit ($T \rightarrow 0$) and approximation at high temperature ($T \rightarrow \infty$)

Quantities	$T \rightarrow 0$	$T \rightarrow \infty$
$\sigma^{(1)}$	$\sigma_0^{(1)}(1+2z)$	$3c_3 k_B T / c_1^2 D \alpha$
σ^2	$\sigma_0^2(1+2z)$	$k_B T / c_1 D \alpha^2$
$\sigma^{(3)}$	$\sigma_0^{(3)}(1+12z)$	$6c_3 (k_B T)^2 / c_1^3 D^2 \alpha^3$
α_T	$\alpha_T^0 z (\ln z)^2 (1+2z)$	α_0^T
$\alpha_T r T \sigma^2 / \sigma^{(3)}$	$3z \ln(1/z) \rightarrow 0$	1/2
$\sigma^{(1)} \sigma^2 / \sigma^{(3)}$	$3(1+2z)^2 / 2(1+12z) \rightarrow 3/2$	1/2

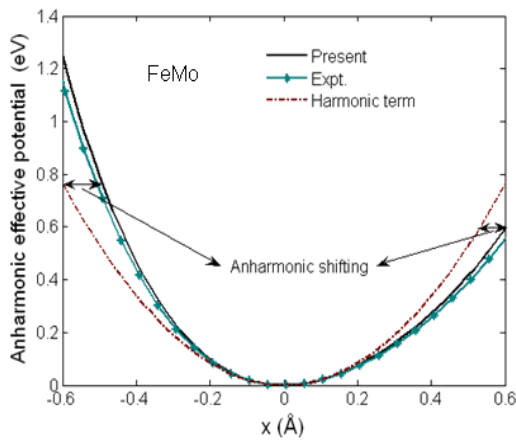


Figure 1: Anharmonic effective interatomic

3. Conclusion

The effective interaction potential in anharmonic correlated Einstein model was determined on base analytics calculation Morse interactive potential between pairs absorber and backscatter atoms with nearest neighbor atoms, this work was reduced the calculation thermodynamic parameters and measures, because replace the calculation by complex matrices three dimensions we only need to solve problem one dimension with the interaction of cluster nearest neighbor atoms and results obtained agree well with experimental data. Figure 1 description anharmonic effective potential interatomic and compared with experimental data for FeMo crystal and graph show the shifts between present theory and experimental data small than shifts between harmonic term with experimentalist, this results to see present procedure can to use good for the study anharmonic vibration of atoms. Figure 2 description the dependence temperature and net expansion of anharmonic perturbation factor in anharmonic correlated Einstein model and form the graph approximate classical at high temperature and quantum effects at low temperature. Figure 3 describe the dependence temperature T of the thermal expansion coefficient, we see α_T approaching the value

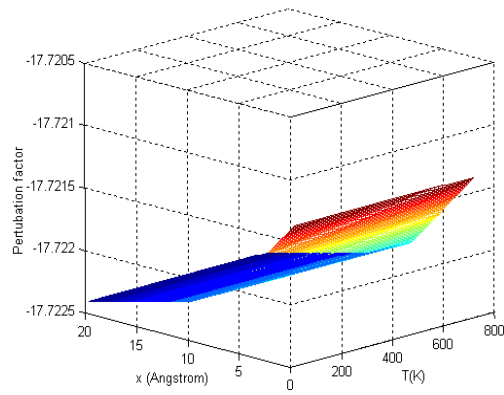


Figure 2: Dependence temperature and net expansion x of anharmonic perturbation factor

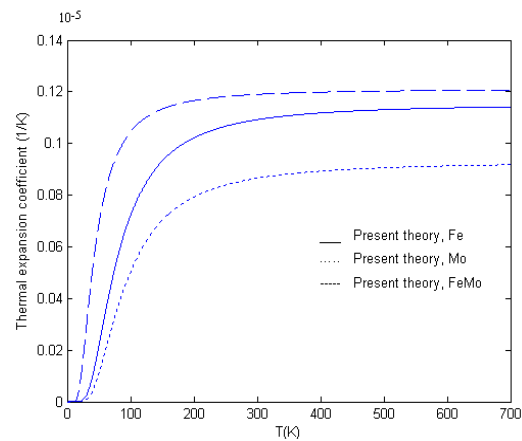


Figure 3: Dependence temperature T of the thermal expansion coefficient α_T

constant α_T^0 at high temperature but has destructed according to exponential at low temperatures.

The thermal expansion coefficient, cumulants and thermodynamic parameters was presented through Debye-Waller factor and structure parameters and has reduced the calculations also measure and programmable calculator. The expression of correlative function between cumulants, correlative function between cumulants and thermal expansion coefficient for cubic structural crystals was determined and inclusion both classical theory at high temperature and quantum effects at low temperature limit.

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