

# Temperature Dependence of High-Order Expanded Anharmonic Correlated Debye Model Debye-Waller Factor of Metallic Copper

Nguyen Bao Trung<sup>1</sup>, Nguyen Van Hung<sup>1, \*</sup>, Ha Dang Khoa<sup>2</sup>

<sup>1</sup>Department of Physics, College of Science, VNU-Hanoi. 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam

<sup>2</sup>School of Engineering Physics, Hanoi University of Science and Technology, 1 Dai Co Viet Road, Hanoi, Vietnam

## Abstract

High-order expanded Debye-Waller factor presented in terms of cumulant expansion in X-ray Absorption Fine Structure (XAFS) of metallic copper, an fcc crystal, has been studied based on anharmonic correlated Debye model. Analytical expressions of dispersion relation, correlated Debye frequency and temperature and four first XAFS cumulants have been derived. Three-dimensional interaction is taken into account in the present one-dimensional model based on the anharmonic effective potential that includes contributions of near neighbors of absorber and backscattering atoms. Numerical results are compared to experiment and found to be in good agreement.

## Keywords

High-Order XAFS Cumulants, Effective Potential, Correlated Debye Model, Metallic Copper

Received: May 17, 2016 / Accepted: May 20, 2016 / Published online: June 1, 2016

© 2016 The Authors. Published by American Institute of Science. This Open Access article is under the CC BY license.

<http://creativecommons.org/licenses/by/4.0/>

## 1. Introduction

X-ray Absorption Fine Structure (XAFS) has developed into a powerful probe of atomic structure and thermal effects of substances [1-13]. XAFS expressions contain Debye-Waller factor presented in terms of cumulant expansion, where the 1<sup>st</sup> cumulant describes the net thermal expansion, the second one describes the mean square relative displacement (MSRD), the 3<sup>rd</sup> and 4<sup>th</sup> cumulants describe anharmonic contributions to XAFS phase and amplitude, respectively [3-10]. The accurate cumulants are crucial to quantitative treatment of anharmonic XAFS. Consequently, the lack of the precise cumulants has been one of the biggest limitations to accurate structural determinations (e.g., the coordination numbers and the atomic distances) from XAFS experiment [2, 3]. Therefore, investigation of XAFS cumulants is of great interest.

The purpose of this work is to derive a method for the calculation and analysis of temperature dependence of XAFS Debye-Waller factor presented in terms of cumulant expansion up to the fourth order of copper (Cu), an fcc crystal describing its thermodynamic properties based on anharmonic correlated Debye model (ACDM). In Sect. 2, the analytical expressions for dispersion relation, correlated Debye frequency and temperature and four first XAFS cumulants of fcc crystals have been derived. They contain more information taken from integration over the phonon wave numbers varied in the 1<sup>st</sup> Brillouin zone (BZ). The three-dimensional interaction is taken into account in the present one-dimensional model based on the anharmonic effective potential [4] that includes contributions of near neighbors of absorber and backscattering atoms. Morse

\* Corresponding author

E-mail address: [trunghpt@yahoo.com](mailto:trunghpt@yahoo.com) (N. B. Trung), [hungnv@vnu.edu.vn](mailto:hungnv@vnu.edu.vn) (N. V. Hung), [khoa.hadang@hust.edu.vn](mailto:khoa.hadang@hust.edu.vn) (H. D. Khoa)

potential is assumed to describe single-pair interatomic interaction included in the effective potential. Numerical results (Sect. 3) are compared to experiment [8, 9] and to those calculated from the single-pair (SP) potential.

## 2. Formalism

To determine the cumulants it is necessary to specify the interatomic potential and force constant [1-13]. In the present theory, a high-order anharmonic interatomic effective potential expanded up to the 4<sup>th</sup> order has been considered

$$V_{eff}(x) \approx \frac{1}{2}k_{eff}x^2 + k_{3eff}x^3 + k_{4eff}x^4, \quad x = r - r_0, \quad (1)$$

where  $k_{eff}$  is effective local force constant,  $k_{3eff}$  and  $k_{4eff}$  are effective anharmonic parameters giving an asymmetry of the anharmonic effective potential,  $x$  is deviation of the instantaneous bond length between two immediate neighboring atoms  $r$  from its equilibrium value  $r_0$ .

The effective potential Eq. (1) is defined based on an assumption in the center-of-mass frame of single bond pair of absorber and backscatterer [4]. For monatomic fcc crystals (Cu) it is given by

$$V_{eff}(x) = V(x) + 2V\left(-\frac{x}{2}\right) + 8V\left(-\frac{x}{4}\right) + 8V\left(\frac{x}{4}\right), \quad (2)$$

where the 1<sup>st</sup> term on the right concerns only absorber and backscatterer atoms and the other ones describe the contributions of remaining neighbors. It is the difference of our effective potential from the SP potential [5, 6] which concerns only each pair of immediate neighboring atoms like  $V(x)$  without remaining terms on the right of Eq. (2).

A Morse potential is assumed to describe the single-pair interatomic interaction contained in the effective potential Eq. (2), and expanded up to the 4<sup>th</sup> order around its minimum

$$V(x) = D(e^{-2\alpha x} - 2e^{-\alpha x}) \approx D\left(-1 + \alpha^2 x^2 - \alpha^3 x^3 + \frac{7}{12}\alpha^4 x^4\right), \quad (3)$$

where  $\alpha$  describes the width of the potential, and  $D$  is dissociation energy.

Applying this Morse potential Eq. (3) to Eq. (2) and comparing to Eq. (1) we determine  $k_{eff}, k_{3eff}, k_{4eff}$  of the anharmonic effective potential in terms of Morse potential parameters.

In the ACDM, the pair model of Eq. (2) is generalized to that of a linear chain with the same effective potential, in order to account for the effects of dispersion. Then, based on [14] for the case of vibration between absorber and backscattering

atoms and using interatomic effective potential for fcc crystals, the dispersion relation is expressed as

$$\omega(q) = 2\alpha\sqrt{\frac{5D}{M}}\left|\sin\left(\frac{qa}{2}\right)\right|, \quad |q| \leq \frac{\pi}{a}, \quad (4)$$

where  $q$  is phonon wave number,  $M$  is mass of composite atoms, and  $a$  is lattice constant.

At the bounds of the 1<sup>st</sup> BZ of the linear chain,  $q = \pm\pi/a$ , the frequency has maximum so that the correlated Debye frequency  $\omega_D$  and temperature  $\theta_D$  have resulted in the following form

$$\omega_D = 2\alpha\sqrt{\frac{5D}{M}}, \quad \theta_D = \frac{\hbar\omega_D}{k_B}, \quad (5)$$

where  $k_B$  is Boltzmann constant.

For calculating XAFS cumulants, we describe the parameter  $x$  in terms of the displacement of  $n$ th atom  $u_n$  of the one-dimensional chain as

$$x_n = u_{n+1} - u_n, \quad (6)$$

where the displacement  $u_n$ 's are related to phonon displacement operators  $A_q$  [15] by

$$u_n = \sqrt{\frac{\hbar}{2NM}} \sum_q \frac{e^{iqan}}{\sqrt{\omega(q)}} A_q, \quad A_q = A_{-q}^\dagger, \quad [A_q, A_{q'}] = 0. \quad (7)$$

Applying  $u_n$  from Eq. (7) to Eq. (6) the parameter  $x_n$  is given by

$$x_n = \sum_q e^{iqan} f(q) A_q, \quad f(q) = \sqrt{\frac{\hbar}{2NM\omega(q)}} (e^{iqa} - 1). \quad (8)$$

In order to include anharmonic effects, Hamiltonian of the system is written in the summation of harmonic and anharmonic components,  $H_0$  and  $H_a$ , respectively

$$H = H_0 + H_a, \quad H_a = H_c + H_q, \quad (9)$$

where  $H_a$  consists of cubic  $H_c$  and quartic  $H_q$  term.

If anharmonic contribution to the anharmonic interatomic effective potential consists of the cubic term, then it can be expressed as

$$H_c = k_{3eff}x^3 = \sum_{q_1, q_2, q_3} V(q_1, q_2, q_3) A_{q_1} A_{q_2} A_{q_3}, \quad (10)$$

or in the following form using Eq. (10) for the displacement of  $n$ th atom

$$H_c = k_{3eff} \sum_n (u_{n+1} - u_n)^3 = k_{3eff} \sum_{q_1, q_2, q_3} \left( \sum_n e^{i(q_1+q_2+q_3)an} \right) f(q_1) f(q_2) f(q_3) A_{q_1} A_{q_2} A_{q_3}. \quad (11)$$

Comparing Eq. (11) to Eq. (10) and indicating

$$\Delta(q) = \frac{1}{N} \sum_n e^{iqna}, \quad \Delta(0) = \sum_n e^{i0na} = N, \quad (12)$$

with N as the atomic number, we obtain

$$V(q_1, q_2, q_3) = k_{3eff} \Delta(q_1 + q_2 + q_3) f(q_1) f(q_2) f(q_3). \quad (13)$$

Using Eq. (8) and Eq. (12), this Eq. (13) changed into

$$V(q_1, q_2, q_3) = k_{3eff} \left( \frac{\hbar}{2NM} \right)^{3/2} \left( \sum_n e^{i(q_1+q_2+q_3)an} \right) \frac{(e^{iq_1a} - 1)(e^{iq_2a} - 1)(e^{iq_3a} - 1)}{\sqrt{\omega(q_1)\omega(q_2)\omega(q_3)}}. \quad (14)$$

The 1<sup>st</sup> cumulant or net thermal expansion has been calculated with the aid of many-body perturbation approach [16] using the expression

$$\sigma^{(1)} = \langle x \rangle = \frac{\sum_q f(q) \langle A_q S(\beta) \rangle_0}{\langle S(\beta) \rangle_0}, \quad (15)$$

$$S(\beta) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_n T[H_a(\tau_1) \dots H_a(\tau_n)],$$

$$\langle x \rangle = - \sum_q f(q) \sum_{q_1, q_2, q_3} V(q_1, q_2, q_3) \int_0^\beta d\tau \langle T[\hat{A}_q(0) \hat{A}_{q_1}(\tau) \hat{A}_{q_2}(\tau) \hat{A}_{q_3}(\tau)] \rangle_0. \quad (18)$$

Using Wick theorem for T-product in the integral, the harmonic phonon Green function [16]

$$G_{q, q'}^0(\tau) = \langle T[\hat{A}_q(\tau) \hat{A}_{q'}(0)] \rangle_0,$$

$$G_{q, q'}^0(\tau) = -\delta_{q, -q'} \left\{ \langle n_q + 1 \rangle e^{-\hbar\omega(q)\tau} + \langle n_q \rangle e^{\hbar\omega(q)\tau} \right\}, \quad (19)$$

the symmetric properties of V(q<sub>1</sub>, q<sub>2</sub>, q<sub>3</sub>) [22], properties of function  $\delta_{q, -q'}$ , the phonon density

$$\langle n_q \rangle = \frac{1}{Z(q) - 1}, \quad Z(q) = \exp(\beta\hbar\omega(q)), \quad \beta = 1/k_B T, \quad (20)$$

as well as  $\omega(q)$  from Eq. (5), f(q) from Eq. (8),  $\Delta(0)$  from Eq. (12) and phonon momentum conservation in the 1<sup>st</sup> BZ, we change further Eq. (18) to the one in terms of Morse parameters. From this expression for large N, the 1<sup>st</sup> cumulant or net thermal expansion has resulted as

$$H_a(t) = e^{tH_0} H_a e^{-tH_0}, \quad (16)$$

with taking backscattering only from the first shell.

Substituting into Eq. (15) the relations [16]

$$\langle A_q S(\beta) \rangle_0 = - \int d\tau \langle T[A_q \hat{H}_1(\tau)] \rangle, \quad \langle A_q \rangle_0 = 0, \quad (17)$$

this equation changed into

$$\sigma^{(1)} = \langle x \rangle = \frac{3a\hbar}{10\pi D\alpha} \int_0^{\pi/a} \omega(q) \frac{1+Z(q)}{1-Z(q)} dq. \quad (21)$$

Now we calculate the second cumulant or MSRD  $\sigma^2$

$$\sigma^{(2)} = \sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 \approx \langle x^2 \rangle. \quad (22)$$

Using Eq. (4) for  $\omega(q)$ , Eq. (8) for  $x_n$  and f(q), Eq. (12) for  $\Delta(q)$  and  $\Delta(0)$ , Eq. (20) for  $G_{q, q'}^0(t)$ , and Eq. (20) for  $\langle n_q \rangle$ , we calculate  $\langle x^2 \rangle$  to obtain the 2<sup>nd</sup> cumulant in terms of Morse parameter. Then, for large N the sum over q is replaced by the corresponding integral and the second cumulant is given by

$$\sigma^2 = \langle x^2 \rangle = \frac{\hbar a}{10\pi D\alpha^2} \int_0^{\pi/a} \omega(q) \frac{1+z(q)}{1-z(q)} dq. \quad (23)$$

The third cumulant has been calculated using the following expression

$$\sigma^{(3)} = \langle x^3 \rangle - 3\langle x^2 \rangle \langle x \rangle + 2\langle x \rangle^3 \approx \langle x^3 \rangle - 3\langle x^2 \rangle \langle x \rangle. \quad (24)$$

The calculation of  $\langle x^3 \rangle$  is analogous to the one of  $\langle x \rangle$  above, i. e.,

$$\langle x^3 \rangle = \frac{\sum_{q_1, q_2, q_3} f(q_1) f(q_2) f(q_3) \langle A_{q_1} A_{q_2} A_{q_3} S(\beta) \rangle_0}{\langle S(\beta) \rangle_0}. \quad (25)$$

Using  $S(\beta)$  from Eq. (16) with limiting only cubic anharmonic term, the Wick theorem for T- product and the

$$F(q_1, q_2) = \frac{\omega(q_1)\omega(q_2)\omega(q_1+q_2)}{\omega(q_1)+\omega(q_2)+\omega(q_1+q_2)} \times \left\{ 1 + 6 \frac{\omega(q_1)+\omega(q_2)}{\omega(q_1)+\omega(q_2)-\omega(q_1+q_2)} \frac{e^{\beta\hbar[\omega(q_1)+\omega(q_2)]} - e^{\beta\hbar\omega(q_1+q_2)}}{(e^{\beta\hbar\omega(q_1)} - 1)(e^{\beta\hbar\omega(q_2)} - 1)(e^{\beta\hbar\omega(q_1+q_2)} - 1)} \right\}. \quad (27)$$

For calculation of the 4<sup>th</sup> cumulant, the Hamiltonian of the system includes anharmonic contributions up to the 4<sup>th</sup> order,

$$H_a = k_{3eff} x^3 + k_{4eff} x^4 = \sum_{q_1, q_2, q_3} V(q_1, q_2, q_3) A_{q_1} A_{q_2} A_{q_3} + \sum_{q_1, q_2, q_3, q_4} V'(q_1, q_2, q_3, q_4) A_{q_1} A_{q_2} A_{q_3} A_{q_4}, \quad (28)$$

$$V'(q_1, q_2, q_3, q_4) = k_{4eff} \left( \frac{\hbar}{2NM} \right)^2 \left( \sum_n e^{i(q_1+q_2+q_3+q_4)an} \right) \frac{(e^{iq_1a} - 1)(e^{iq_2a} - 1)(e^{iq_3a} - 1)(e^{iq_4a} - 1)}{\sqrt{\omega(q_1)\omega(q_2)\omega(q_3)\omega(q_4)}}. \quad (29)$$

The 4<sup>th</sup> cumulant has been calculated based on the following expression

$$\sigma^{(4)} = \langle x^4 \rangle - 4\langle x^3 \rangle \langle x \rangle - 3\langle x^2 \rangle^2 + 12\langle x^2 \rangle \langle x \rangle^2 - 6\langle x \rangle^4 \approx \langle x^4 \rangle - 3\langle x^2 \rangle^2. \quad (30)$$

Calculation of  $\langle x^4 \rangle$  is analogous to the one of  $\langle x \rangle$  above, using  $\langle x^2 \rangle$  from Eq. (22) we obtain  $3\langle x^2 \rangle^2$ . Substituting these values into Eq. (30) and using the phonon momentum

$$\sigma^{(4)} = \frac{24.94 \times 10^{-4} \hbar^3 a^3}{\pi^3 D^3 \alpha^4} \int_0^{\pi/a} dq_1 \int_0^{\pi/a-q_1} dq_2 \int_{-\pi/a}^{\pi/a-(q_1+q_2)} dq_3 \frac{\omega(q_1)\omega(q_2)\omega(q_3)\omega(q_4)}{\omega(q_1)+\omega(q_2)+\omega(q_3)+\omega(q_4)} \times \left\{ 1 + 8 \frac{Z(q_1)Z(q_2)Z(q_3) - Z(q_4)}{(Z(q_1)-1)(Z(q_2)-1)(Z(q_3)-1)(Z(q_4)-1)} \frac{\omega(q_1)+\omega(q_2)+\omega(q_3)}{\omega(q_1)+\omega(q_2)+\omega(q_3)-\omega(q_4)} + 6 \frac{Z(q_1)Z(q_2) - Z(q_3)Z(q_4)}{(Z(q_1)-1)(Z(q_2)-1)(Z(q_3)-1)(Z(q_4)-1)} \frac{\omega(q_3)+\omega(q_4)}{\omega(q_1)+\omega(q_2)-\omega(q_3)-\omega(q_4)} \right\} \quad (31)$$

### 3. Numerical Results and Discussions

Now the expressions derived in the previous section are

symmetric properties of  $V(q_1, q_2, q_3)$  [22], we calculated  $\langle x^3 \rangle$  of Eq. (25). The product  $3\langle x^2 \rangle \langle x \rangle$  has been calculated using  $\langle x^2 \rangle$  from Eq. (22) and  $\langle x \rangle$  from Eq. (21).

Substituting the obtained  $\langle x^3 \rangle$  and  $3\langle x^2 \rangle \langle x \rangle$  into Eq. (25) with application of the relation for phonon momentum conservation in the first BZ we obtain the 3<sup>rd</sup> cumulant  $\sigma^{(3)}$  in terms of Morse parameters. Then, for large N the summation over  $q$  can be replaced by the corresponding integral and it is given by

$$\sigma^{(3)} = \frac{5\hbar^2 a^2}{200N^2 \pi^2 D^2 \alpha^3} \int_0^{\pi/a} dq_1 \int_{-\pi/d}^{\pi/a-q_1} dq_2 F(q_1, q_2), \quad (26)$$

so that similar to Eq. (11) we obtain

conservation in the first BZ, the 4<sup>th</sup> cumulant Eq. (30) in terms of Morse parameters has resulted. Then, for large N the summation over  $q$  can be replaced by the corresponding integral and it is given by

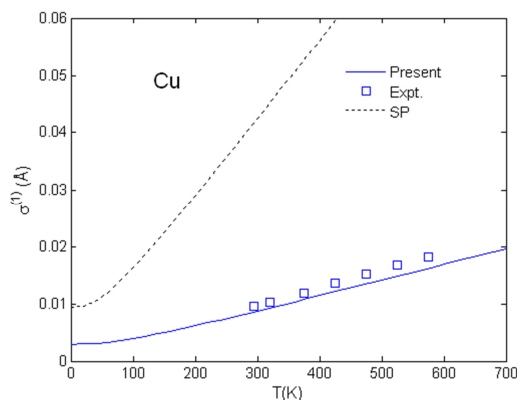
applied to numerical calculations for Cu using its Morse parameters [17]  $D = 0.337$  eV,  $\alpha = 1.358$  Å<sup>-1</sup>. Some calculated results of the local force constant  $k_S$ , anharmonic potential parameters  $k_{3S}$ ,  $k_{4S}$ , correlated Debye frequency

$\omega_{DS}$  and temperature  $\theta_{DS}$  for the anharmonic effective (S = *eff*), and single pair (S = SP) potentials are written in Table 1. They show good agreement of the results calculated using the present theory (S = *eff*) with experiment (S = Expt.) [8] and significant differences from those calculated using the SP potential.

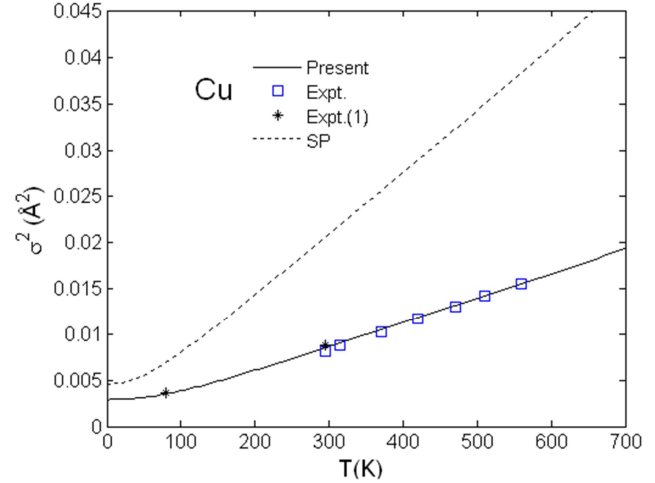
**Table 1.** The values of  $k_S, \omega_{DS}, \theta_{DS}$  of Cu calculated using the present theory with effective (S = *eff*) potential compared to experiment (S = Expt.) and to those calculated using the single-pair (S = SP) potential.

S	$k_S (N/m)$	$\omega_{DS} (\times 10^{13} Hz)$	$\theta_{DS} (K)$
<i>eff</i> (Present)	50.7181	4.3717	333.9399
Expt. [8]	50.3450	4.3556	332.7094
SP	20.2872	2.7649	211.2021

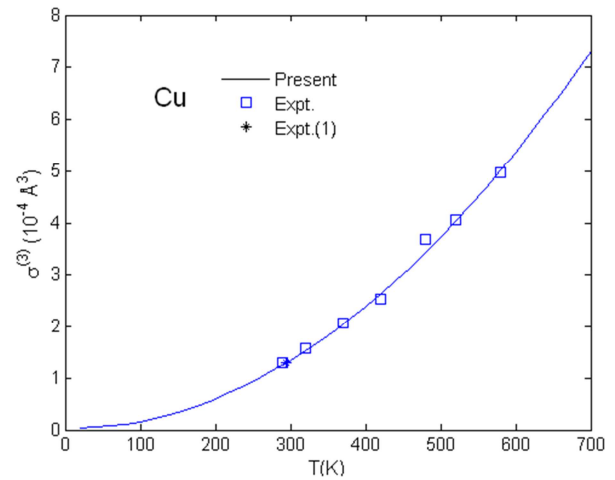
Temperature dependence of 1<sup>st</sup> cumulant or net thermal expansion  $\sigma^{(1)}(T)$  calculated using the present theory (Fig. 1) is found to be in reasonable agreement with experiment [8]. Temperature dependence of 2<sup>nd</sup> cumulant or MSRD  $\sigma^2(T)$  calculated using the present theory (Fig. 2) agrees well with the experimental values [8, 9]. Both they are quite different from the results calculated using the SP potential. Good agreement with the experimental values [8, 9] has been also obtained for temperature dependence of 3<sup>rd</sup> cumulant  $\sigma^{(3)}(T)$  (Fig. 3) and 4<sup>th</sup> cumulant  $\sigma^{(4)}(T)$  (Fig. 4) calculated using the present theory. These results of  $\sigma^{(3)}(T)$  and  $\sigma^{(4)}(T)$  are also quite different from those calculated using the SP potential as it was illustrated for  $\sigma^{(1)}(T)$  (Fig. 1) and  $\sigma^2(T)$  (Fig. 2), but we do not show them in Figs. 3 and 4, respectively. Hence, the results calculated using the present theory based on the anharmonic effective potential overcome significant discrepancies with experiment shown in those calculated using the SP potential presented in Figs. 1



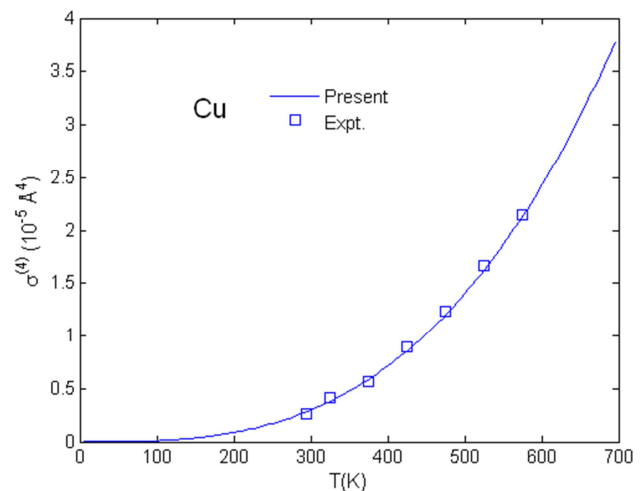
**Fig. 1.** Temperature dependence of 1<sup>st</sup> cumulant or net thermal expansion  $\sigma^{(1)}(T)$  of Cu calculated using the present theory compared to the experimental values Expt. [8] and to those calculated using the SP potential.



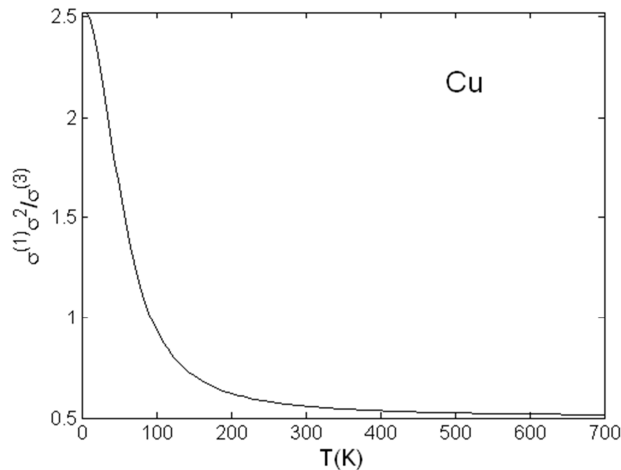
**Fig. 2.** Temperature dependence of 2<sup>nd</sup> cumulant or MSRD  $\sigma^2(T)$  of Cu calculated using the present theory compared to the experimental values Expt. [8], Expt.(1) [9] and to those calculated using the SP potential.



**Fig. 3.** Temperature dependence of 3<sup>rd</sup> cumulant  $\sigma^{(3)}(T)$  of Cu calculated using the present theory compared to the experimental values Expt. [8] and Expt.(1) [9].



**Fig. 4.** Temperature dependence of 4<sup>th</sup> cumulant  $\sigma^{(4)}(T)$  of Cu calculated using the present theory compared to the experimental values Expt. [8].



**Fig. 5.** Temperature dependence of cumulant ratio  $\sigma^{(1)}\sigma^2/\sigma^{(3)}$  of Cu calculated using the present theory.

and 2. Such discrepancies can be attributed to neglecting the three-dimensional interaction in the SP potential.

Note that the above calculated results confirm the proportionality of the 1<sup>st</sup> and 2<sup>nd</sup> cumulants to the temperature  $T$ , the 3<sup>rd</sup> and 4<sup>th</sup> cumulants to  $T^2$  and  $T^3$ , respectively at high-temperatures, as well as their containing zero-point energy contributions at low-temperatures, a quantum effect.

Cumulant ratio is often considered as a standard in XAFS theory to identify the temperature above which the cumulant ratio approaches the constant value of 1/2 so that the classical limit is applicable [4, 5]. Fig. 5 illustrates temperature dependence of the cumulant ratio  $\sigma^{(1)}\sigma^2/\sigma^{(3)}$  of Cu calculated using the present theory. This temperature for the present ACDM of Cu is about the Debye temperature  $\theta_D = 334$  K (Tab. 1) instead of the Einstein temperature for the anharmonic correlated Einstein model (ACEM) [4].

## 4. Conclusions

In this work a method has been derived for the calculation and analysis of temperature dependence of high-order expanded XAFS Debye-Waller factor presented in terms of cumulant expansion up to the fourth order for metallic Cu based on the ACDM. The three-dimensional interaction has been taken into account in the present one-dimensional model based on the anharmonic effective potential which includes the contributions of all nearest neighbors of absorber and backscattering atoms. The present method can also be generalized to study the other fcc metals.

The derived expressions for the anharmonic effective potential, dispersion relation, correlated Debye frequency and temperature, as well as the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup> and 4<sup>th</sup> XAFS cumulants satisfy all their fundamental properties where the present theory cumulants overcome significant discrepancies with experiment of the results calculated using the SP

potential.

The good agreement of numerical results for Cu with experiment illustrates the advantages and efficiency of the present theory and of using the anharmonic effective potential in XAFS data analysis.

## Acknowledgements

The authors thank Prof. J. J. Rehr and Prof. P. Fornasini for useful comments.

## References

- [1] Crozier E. D.; J. J. Rehr J. J.; Ingalls R. X-ray Absorption. Edited by D. C. Koningsberger and R. Prins (Wiley, New York, 1988). Chap. 9.
- [2] Vila F. D.; Rehr J. J.; Rossner H. H.; Krappe H. J. Theoretical x-ray absorption fine structure Debye-Waller factors. *Phys. Rev. B* 2007, 76, 014301.
- [3] Hung N. V.; Tien T. S.; Duc N. B.; Vuong D. Q. High-order expanded XAFS Debye-Waller factors of hcp crystals based on classical anharmonic correlated Einstein model. *Mod. Phys. Lett. B* 2014, 28, 1450174.
- [4] Hung N. V.; Rehr J. J. Anharmonic correlated Einstein model Debye-Waller factors. *Phys. Rev. B* 1997, 56, 43.
- [5] Frenkel A. I.; Rehr J. J. Thermal expansion and x-ray absorption fine-structure cumulants. *Phys. Rev. B* 1993, 48, 585.
- [6] Miyanaga T.; Fujikawa T. Quantum Statistical Approach to Debye-Waller Factor in EXAFS, EELS and ARXPS. III. Application of Debye and Einstein Approximation. *J. Phys. Soc. Jpn.* 1994, 63, 3683.
- [7] Daniel M.; Pease D. M.; Hung N. V.; Budnick J. D. Local force constants of transition metal dopants in a nickel host: Comparison to Mossbauer studies. *Phys. Rev. B* 2004, 68, 134414.
- [8] Pirog I. V.; Nedoseikina T. I.; Zarubin A. I.; Shuvaev A. T. Anharmonic pair potential study in face-centered cubic crystals. *J. Phys.: Condens. Matter* 2002, 14, 1825.
- [9] Yokoyama T.; Sasukawa T.; Ohta T. Anharmonic Interatomic Potentials of Metals and Metal Bromides Determined by EXAFS. *Jpn. J. Appl. Phys.* 1989, 28, 1905.
- [10] Fornasini P. and Grisenti R. On EXAFS Debye-Waller factor and recent advances. *J. Synch. Rad.* 2015, 22, 1242.
- [11] Hung N. V.; Tien T. S.; Hung L. H.; Frahm R. R. Anharmonic Effective Potential, Local Force Constant and EXAFS of HCP Crystals: Theory and Comparison to Experiment. *Int. J. Mod. Phys. B* 2008, 22, 5155.
- [12] Hung N. V.; Hung V. V.; Hieu H. K.; Frahm R. R. Pressure effects in Debye-Waller factors and in EXAFS. *Physica B* 2011, 406, 456.
- [13] Hung N. V.; Thang C. S.; Toan C. T.; Hieu H. K. Temperature dependence of Debye-Waller factors of semiconductors. *Vacuum* 2014, 101, 63-66.

- [14] Kittel C. Introduction to Solid State Physics (John-Wiley&Sons, Inc., New York, 1986), 6<sup>th</sup> ed.
- [15] Maradudin A. A. Dynamical Properties of Solids, ed. by G. K. Horton and A. A. Maradudin (North Holland, Amsterdam, 1974) Vol. 1, p. 1.
- [16] Mahan G. D. Many-Particle Physics (Plenum, New York, 1990) 2<sup>nd</sup> ed.
- [17] Girifalco L. A.; Weizer W. G. Application of the Morse Potential Functions to Cubic Metals. Phys. Rev. 1959, 114, 687.