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# High-Order XAFS Cumulants of fcc Crystals Based on Anharmonic Correlated Debye Model and Effective Potential

Nguyen Van Hung<sup>1</sup>, Nguyen Bao Trung<sup>1</sup>, Nguyen Ba Duc<sup>2</sup>, Duong Duy Son<sup>1</sup> and Tong Sy Tien<sup>1</sup>

1. Department of Physics, Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Vietnam

2. Tan Trao University, Km 6, Trung Mon, Yen Son, Tuyen Quang, Vietnam

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**Abstract:** High-order cumulants of fcc crystals in X-ray absorption fine structure (XAFS) have been studied based on anharmonic correlated Debye model and anharmonic effective potential. Analytical expressions for dispersion relation, correlated Debye frequency and temperature, first, second, third and fourth cumulants have been derived which involve more information of phonons taken from integration over the first Brillouin zone. Derived anharmonic effective potential includes contributions of all nearest neighbors of absorber and backscattering atoms to take into account three-dimensional interaction. Morse potential is used to describe interaction between each pair of atoms. Numerical results for Cu are found to be in good agreement with experiment.

**Key words:** High-order XAFS cumulants, effective potential, correlated Debye model, fcc crystals.

## 1. Introduction

Thermal vibrations and disorder in XAFS give rise to Debye-Waller factors (DWFs) varying as  $e^{-W(Q)}$ , which are presented in terms of cumulant expansion [1] where the even cumulants contribute to the amplitude and the odd ones to the phase of XAFS. 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. Therefore, investigation of XAFS cumulants is of great interest.

Many efforts have been made to calculate the cumulants for including anharmonic effects or phonon-phonon interactions in temperature dependent XAFS. At high temperatures the classical approach can work well [2-7]. But it cannot be valid at low

temperatures due to zero-point vibration [8-11]. Several approaches have been derived to calculate the XAFS cumulants such as full lattice dynamical (FLD) approach [8] using single pair (SP) potential, single-bond (SB) model [9], anharmonic correlated Einstein model (ACEM) [10], path integral calculation [11], force constant (FC) theory [12], and statistical moment method for DWFs of semiconductors [13], etc.. They have achieved excellent steps in studying anharmonic XAFS. The fourth cumulant is important as an anharmonic contribution to XAFS amplitude [6] and has been measured for some crystals [14-16]. The ACEM [10] has been successfully applied to calculating cumulants and XAFS for fcc crystals [10, 17-20], but it is limited only to the third cumulant and without considering dispersion relations.

Our development in this work is to derive a method for the calculation and analysis of high-order XAFS cumulants of fcc crystals based on anharmonic correlated Debye model (ACDM) and anharmonic

**Corresponding author:** Nguyen Van Hung, Ph.D., professor, research fields: solid state physics and XAFS theory. E-mail: hungnv@vnu.edu.vn.

effective potential. 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 involve more information taken from integration over phonon wave numbers varied in the first Brillouin zone (BZ). Anharmonic effective potential expanded up to fourth order includes contributions of all nearest neighbors of absorber and backscattering atoms to take into account three-dimensional interactions. Numerical results for Cu (Sect. 3) are found to be in good agreement with experiment [14-16] and show some advantages compared to the single-pair (SP) potential procedure.

## 2. Formalism

### 2.1 High-Order Anharmonic Effective Potential

To determine XAFS cumulants it is necessary to specify the interatomic interaction potential and local force constant [4-20]. It is considered that a high-order anharmonic interatomic effective potential expanded to the fourth order around its minimum:

$$V_{eff}(x) \approx \frac{1}{2}k_{eff}x^2 + k_3x^3 + k_4x^4, \quad x = r - r_0 \quad (1)$$

where,  $k_{eff}$  is effective local force constant,  $k_3$  and  $k_4$  are anharmonic parameters giving an asymmetry of anharmonic effective potential,  $x$  is deviation of 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 atoms [11]. For monatomic fcc crystals 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 first term on the right concerns only absorber and backscatterer atoms, the remaining terms describe contributions of nearest neighbors. It is the difference of our effective potential Eq. (2) from the SP potential [8, 9] which concerns only each pair of the immediate neighboring atoms like  $V(x)$  without

remaining terms.

A Morse potential is assumed to describe interaction between each pair of atoms contained in the effective potential Eq. (2), and expanded to the fourth order around its minimum:

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

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

Applying this Morse potential Eq. (3) to Eq. (2) and comparing the result to Eq. (1) the anharmonic effective potential parameters  $k_{eff}$ ,  $k_3$  and  $k_4$  in terms of Morse parameters are determined.

### 2.2 Dispersion Relation, Correlated Debye Frequency and Temperature

Based on ACDM we generalize the pair model of Eq. (2) to that of a linear chain with the same effective potential in order to account for the effects of dispersion. Then according to [21] for the case of vibration between absorber and backscattering atoms and using our 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 first BZ of the linear chain,  $q = \pm\pi/a$ , the frequency has maximum so that we get correlated Debye frequency  $\omega_D$  and temperature  $\theta_D$ :

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

where,  $k_B$  is Boltzmann constant.

### 2.3 Derivation of 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 the phonon displacement operators  $A_q$  [22] by:

$$u_n = \sqrt{\frac{\hbar}{2NM}} \sum_q \frac{e^{iqan}}{\sqrt{\omega(q)}} A_q$$

$$A_q = A_{-q}^\dagger, [A_q, A_{q'}] = 0 \quad (7)$$

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

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

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

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

where,  $H_a$  consists of cubic  $H_c$  and quartic  $H_q$  terms.

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

$$H_c = k_3 x^3 = \sum_{q_1, q_2, q_3} V(q_1, q_2, q_3) A_{q_1} A_{q_2} A_{q_3} \quad (10)$$

or in the following form using Eq. (7) for the displacement of  $n$ th atom:

$$H_c = k_3 \sum_n (u_{n+1} - u_n)^3 = k_3 \sum_{q_1, q_2, q_3} \left( \sum_n e^{i(q_1+q_2+q_3)an} \right) \times$$

$$\times f(q_1) f(q_2) f(q_3) A_{q_1} A_{q_2} A_{q_3} \quad (11)$$

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

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

with  $N$  as the atomic number we obtain:

$$V(q_1, q_2, q_3) = k_3 \Delta(q_1 + q_2 + q_3) f(q_1) f(q_2) f(q_3) \quad (13)$$

which by using Eq. (8) and Eq. (12) is changed into:

$$V(q_1, q_2, q_3) = k_3 \left( \frac{\hbar}{2NM} \right)^{3/2} \left( \sum_n e^{i(q_1+q_2+q_3)an} \right)$$

$$\times \frac{(e^{iq_1a} - 1)(e^{iq_2a} - 1)(e^{iq_3a} - 1)}{\sqrt{\omega(q_1)\omega(q_2)\omega(q_3)}} \quad (14)$$

The 1st cumulant or net thermal expansion has been calculated with the aid of many-body perturbation approach [23] using the expression:

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

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

$$H_a(t) = e^{iH_0} H_a e^{-iH_0} \quad (16)$$

with taking backscattering only from the first shell.

Substituting into Eq. (15) the relations [23]:

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

we obtain:

$$\langle x \rangle = - \sum_q f(q) \sum_{q_1, q_2, q_3} V(q_1, q_2, q_3) \times$$

$$\times \int_0^\beta d\tau \langle T[\hat{A}_q(0) \hat{A}_{q_1}(\tau) \hat{A}_{q_2}(\tau) \hat{A}_{q_3}(\tau)] \rangle_0 \quad (18)$$

Using Wick theorem for T-product in the integral, the harmonic phonon Green function [23]:

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

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

the symmetric properties of  $V(q_1, q_2, q_3)$  [22], the properties of function  $\delta_{q,-q}$ , the phonon density:

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

as well as  $\omega(q)$  of Eq. (4),  $f(q)$  of Eq. (8),  $\Delta(0)$  of Eq. (12) and phonon momentum conservation in the 1st BZ, Eq. (18) is changed further into:

$$\langle x \rangle = \frac{3\hbar\alpha\sqrt{\alpha}}{4N\sqrt{5MD}} \sum_q \sin \frac{qa}{2} \frac{1 + Z(q)}{1 - Z(q)} \quad (21)$$

For large  $N$ , the sum over  $q$  can be replaced by the corresponding integral, so that the 1st cumulant has resulted as:

$$\sigma^{(1)} = \langle x \rangle = \frac{3a\hbar}{10\pi D\alpha} \int_0^{\pi/a} \omega(q) \frac{1 + Z(q)}{1 - Z(q)} dq \quad (22)$$

Now we calculate the 2nd cumulant equaling mean square relative displacement (MSRD)  $\sigma^2$ :

$$\sigma^{(2)} = \sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 \approx \langle x^2 \rangle \quad (23)$$

Using Eq. (4) for  $\omega(q)$ , Eq. (8) for  $x_n$  and  $f(q)$ , Eq. (12) for  $\Delta(q)$  and  $\Delta(0)$ , Eq. (19) for  $G_{q,q}^0(t)$ , and Eq. (21) for  $\langle n_q \rangle$  we calculate  $\langle x^2 \rangle$  to obtain the 2nd cumulant in terms of Morse parameters:

$$\sigma^2 = \langle x^2 \rangle = \frac{\hbar}{N\alpha\sqrt{5MD}} \sum_q \left| \sin \frac{qa}{2} \frac{1+Z(q)}{1-Z(q)} \right| \quad (24)$$

This equation for large N is changed into:

$$\sigma^2 = \frac{\hbar a}{10\pi D \alpha^2} \int_0^{\pi/a} \omega(q) \frac{1+z(q)}{1-z(q)} dq = \frac{\sigma^{(1)}}{3\alpha} \quad (25)$$

which is proportional to the 1st cumulant as in the ACEM [11].

The 3rd cumulant has been calculated using the following expression:

$$\sigma^{(3)} \approx \langle x^3 \rangle - 3\langle x^2 \rangle \langle x \rangle \quad (26)$$

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

$$\langle x^3 \rangle = \frac{\sum_{q_1, q_2, q_3} f(q_1)f(q_2)f(q_3) \langle A_{q_1} A_{q_2} A_{q_3} S(\beta) \rangle_0}{\langle S(\beta) \rangle_0} \quad (27)$$

Using  $S(\beta)$  from Eq. (16) with limiting only cubic anharmonic term, the Wick theorem for T-product and the symmetric properties of  $V(q_1, q_2, q_3)$  [22], we calculate  $\langle x^3 \rangle$ . The product  $3\langle x^2 \rangle \langle x \rangle$  has been calculated using  $\langle x^2 \rangle$  from Eq. (24) and  $\langle x \rangle$  from Eq. (21). Substituting them into Eq. (27) with application of the relation for phonon momentum conservation in the 1st BZ, we obtain the 3rd cumulant in terms of Morse parameters which for large N is given by:

$$\sigma^{(3)} = \frac{5\hbar^2 a^2}{200N^2 \pi^2 D^2 \alpha^3} \int_0^{\pi/a} dq_1 \int_{-\pi/d}^{\pi/a-q_1} dq_2 F(q_1, q_2) \quad (28)$$

$$F(q_1, q_2) = \frac{\omega(q_1)\omega(q_2)\omega(q_1+q_2)}{\omega(q_1)+\omega(q_2)+\omega(q_1+q_2)} \times$$

$$\times \left\{ 1 + 6 \frac{\omega(q_1)+\omega(q_2)}{\omega(q_1)+\omega(q_2)-\omega(q_1+q_2)} \times$$

$$\left. \frac{e^{\beta\hbar[\omega(q_1)+\omega(q_2)]} - e^{\beta\hbar\omega(q_1+q_2)}}{(e^{\beta\hbar\omega(q_1)} - 1)(e^{\beta\hbar\omega(q_2)} - 1)(e^{\beta\hbar\omega(q_1+q_2)} - 1)} \right\} \quad (29)$$

For calculating the 4th cumulant, the Hamiltonian of the system includes anharmonic contributions up to the 4th order, so that similar to Eq. (11) we obtain the anharmonic component:

$$H_a = \sum_{q_1, q_2, q_3} V(q_1, q_2, q_3) A_{q_1} A_{q_2} A_{q_3} + \sum_{q_1, q_2, q_3, q_4} V'(q_1, q_2, q_3, q_4) A_{q_1} A_{q_2} A_{q_3} A_{q_4} \quad (30)$$

$$V'(q_1, q_2, q_3, q_4) = k_4 \left( \frac{\hbar}{2NM} \right)^2 \left( \sum_n e^{i(q_1+q_2+q_3+q_4)an} \right) \times$$

$$\times \frac{(e^{iq_1a} - 1)(e^{iq_2a} - 1)(e^{iq_3a} - 1)(e^{iq_4a} - 1)}{\sqrt{\omega(q_1)\omega(q_2)\omega(q_3)\omega(q_4)}} \quad (31)$$

The 4th cumulant has been calculated based on the following expression:

$$\sigma^{(4)} \approx \langle x^4 \rangle - 3\langle x^2 \rangle^2 \quad (32)$$

Calculation of  $\langle x^4 \rangle$  is analogous to the one of  $\langle x \rangle$  above, using  $\langle x^2 \rangle$  from Eq. (24), we obtain  $3\langle x^2 \rangle^2$ . Substituting these values into Eq. (32) and using the phonon momentum conservation in the first BZ, the 4th cumulant Eq. (32) in terms of Morse parameters has been calculated which for large N is given by:

$$\sigma^{(4)} = \frac{24.94 \times 10^{-4} \hbar^3 a^3}{\pi^3 D^3 \alpha^4} \int_0^{\pi/a} dq_1 \int_0^{\pi/a-q_1} dq_2 \int_{-\pi/a}^{\pi/a-(q_1+q_2)} dq_3 F(q_1, q_2, q_3, q_4) \quad (33)$$

$$F(q_1, q_2, q_3, q_4) = \frac{\omega(q_1)\omega(q_2)\omega(q_3)\omega(q_4)}{\omega(q_1)+\omega(q_2)+\omega(q_3)+\omega(q_4)} \times$$

$$\left\{ 1 + 8 \frac{Z(q_1)Z(q_2)Z(q_3) - Z(q_4)}{(Z(q_1)-1)(Z(q_2)-1)(Z(q_3)-1)(Z(q_4)-1)} \times$$

$$\times \frac{\omega(q_1)+\omega(q_2)+\omega(q_3)}{\omega(q_1)+\omega(q_2)+\omega(q_3)-\omega(q_4)}$$

$$+ 6 \frac{Z(q_1)Z(q_2) - Z(q_3)Z(q_4)}{(Z(q_1)-1)(Z(q_2)-1)(Z(q_3)-1)(Z(q_4)-1)} \times$$



$$\times \frac{\omega(q_3) + \omega(q_4)}{\omega(q_1) + \omega(q_2) - \omega(q_3) - \omega(q_4)} \} \quad (34)$$

### 3. Numerical Results and Discussion

Now we apply the expressions derived in previous sections to numerical calculations for Cu using its calculated Morse parameters (CMP)  $D = 0.3429$  eV,  $\alpha = 1.3588 \text{ \AA}^{-1}$  [24]. Debye temperature calculated by the present theory using CMP [24]  $\theta_D = 333$  K and the one obtained from its measured Morse parameters (MMP) [14]  $\theta_D = 332$  K are close to experimental values 323 K [15] and 315 K [25]. They are quite different from  $\theta_D = 211$  K calculated using SP potential. The anharmonic effective potential (Fig. 1a) and dispersion relation (Fig. 1b) of Cu calculated using CMP [24] coincide with those obtained from MMP [15] and are quite different from those of the SP potential calculated using CMP. Temperature dependence of our calculated 2nd cumulant or DWF  $\sigma^2(T)$  (Fig. 2) agrees well with experiment [14, 15] and is quite different from the one calculated using SP potential. Temperature dependence of the 3rd (Fig. 3a) and 4th (Fig. 3b) cumulant agrees well with experiment [14, 16] and is also quite different from those calculated by SP potential which is shown only in Fig. 2 for 2nd cumulant as an example. Hence, the results calculated by the present theory using our anharmonic effective potential have advantages compared to those calculated using the SP potential [8] shown by better agreement of our results with experiment.

Cumulant relation is often considered as a standard for cumulant calculation and measurement [6, 11, 19].

Fig. 4 shows temperature dependence of cumulant relation  $\sigma^{(1)}\sigma^2/\sigma^{(3)}$  calculated using the present theory for Cu. It approaches the constant value of 1/2 at high-temperature satisfying the condition obtained from experiment [6], classical [6] and quantum [10, 19] theory. Then it also can be considered as the standard for cumulant study using ACDM.

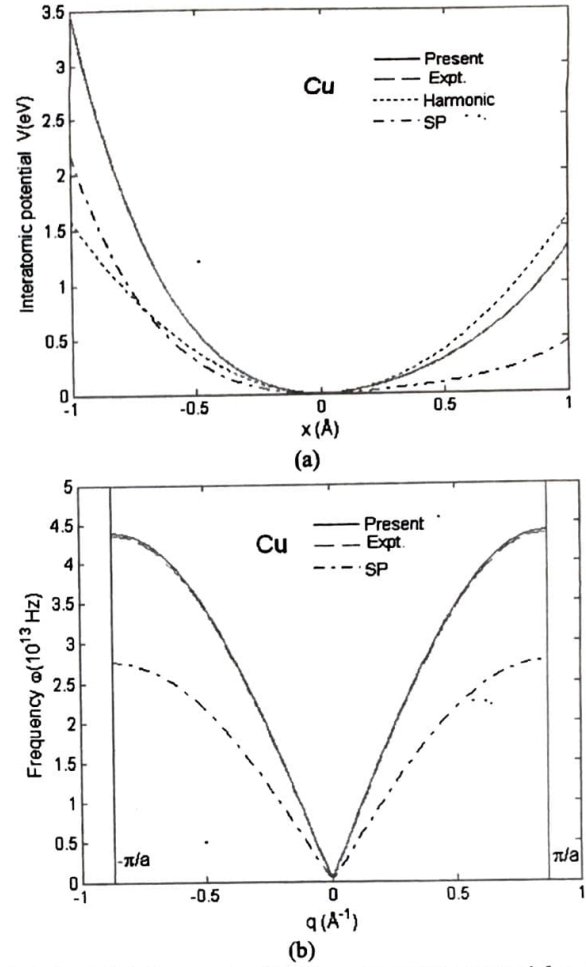


Fig. 1 (a) Anharmonic effective interatomic potential and (b) dispersion relation calculated using CMP [24] compared to those (Expt.) obtained from MMP [14] and to the result calculated by SP potential using CMP.

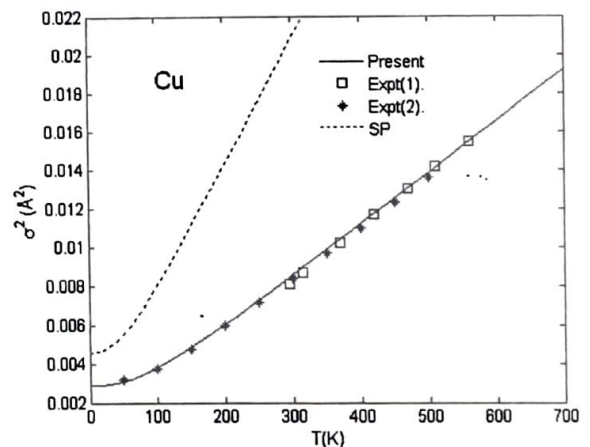


Fig. 2 Temperature dependence of our calculated 2nd cumulant  $\sigma^2(T)$  compared to experiment Expt (1) [14] and Expt (2) [15] and to that calculated using SP potential.

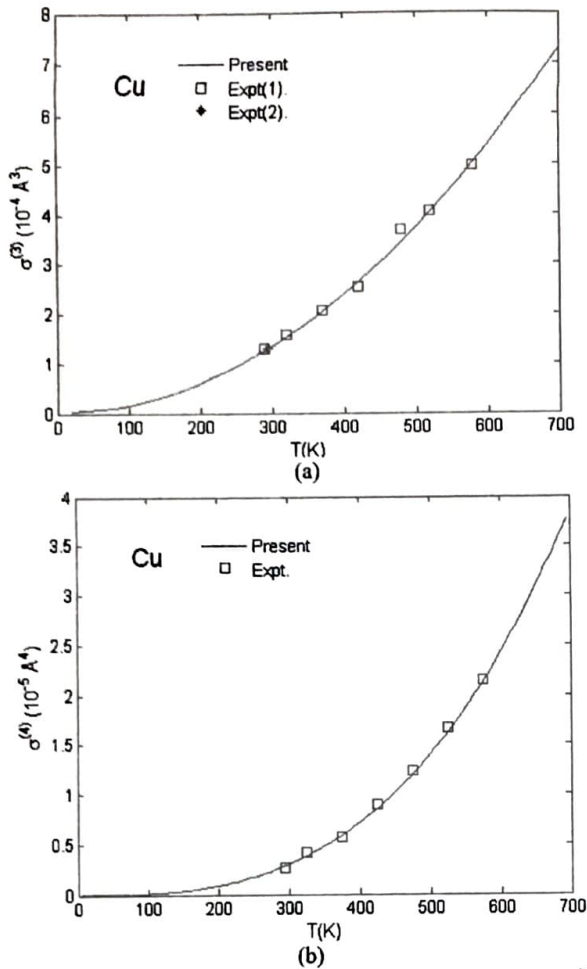


Fig. 3 Temperature dependence of our calculated (a) 3<sup>rd</sup> cumulant  $\sigma^{(3)}(T)$  and (b) 4<sup>th</sup> cumulant  $\sigma^{(4)}(T)$  of Cu compared to experiment Expt.(1) [14] and Expt.(2) [16] for  $\sigma^{(3)}(T)$ , as well as to Expt. [14] for  $\sigma^{(4)}(T)$ .

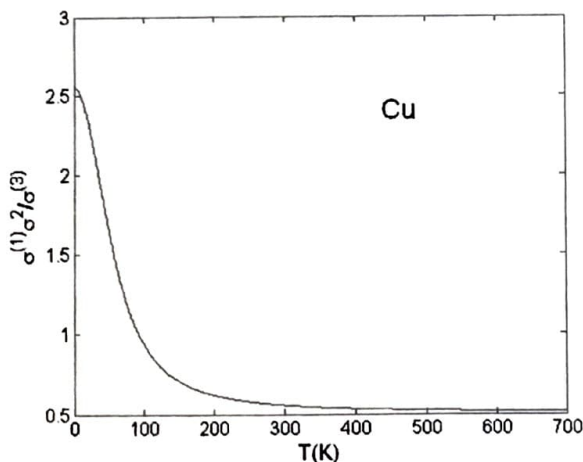


Fig. 4 Temperature dependence of cumulant relation  $\sigma^{(1)}\sigma^2/\sigma^{(3)}$  for Cu calculated using the present theory.

## 4. Conclusions

A method has been derived for the calculation and analysis of high-order XAFS cumulants of fcc crystals based on ACDM which considers dispersion relation to take more information of phonons taken from integration over the 1st BZ and anharmonic effective potential to take into account three-dimensional interaction, where Morse potential is used for describing interaction between each pair of atoms.

Derived expressions for the above considered quantities satisfy all their fundamental properties in temperature dependence and provide better agreement with experiment compared to those calculated using SP potential.

The good agreement of our 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.

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