Temperature dependence of the correlation function in EXAFS spectra: Application to Cu-Ag alloys

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Temperature dependence of the correlation function in EXAFS spectra: Application to Cu-Ag alloys

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Abstract. Correlation ratios between the mean square displacement (MSD), mean square relative displacement (MSRD), and correlated displacement function were studied in extended X-ray absorption fine structure spectra (EXAFS). The expressions of MSD, MSRD, and correlation function were determined using Debye models. Hardy problems due to many-particles effects were considered and replaced by a calculation based on the effective anharmonic potential, including the interaction of absorbing and scattering atoms with their nearest neighbours atoms. Based on the Debye-Waller factor, the difference between MSRD and MRD was analyzed, and their ratios have calculated. The methods were applied to fcc crystals and their alloys. Numerical results for Cu, Ag crystals and CuAg50 alloys agreed with experimental values and other studies.
Keywords: Anharmonic effective potential; Correlated displacement function; Correlation ratio; Debye-Waller factor; Mean square displacement.

1. Introduction

In the harmonic approximation, extended X-ray absorption fine structure (EXAFS) is usually written form;

$$\chi(\kappa) = \sum_j \frac{S_0^2(\kappa) N_j}{\kappa \Re_j^2} F_j(\kappa) e^{-2\sigma_j^2 \kappa^2} e^{-2\Re_j/\lambda} \sin[2\kappa\Re_j + \delta_j(\kappa)], \quad (1)$$

where S_0^2, N_j, $F(\kappa)$, $\delta(\kappa)$, $\Re_j$, κ and λ have been defined [2], [5]. The factor in the exponential function of the Eq.(1) $Z(T) = 2\sigma_j^2\kappa^2(T)$ is the Debye-Waller factor (DWF), $\sigma^2(T)$ in Mean Square Relative Displacement (MSRD) of the bond between two nearest atoms [7]. During the diffraction of neutrons or X-ray absorption, the DWF has a similar form $Z(T) = (1/2)\sigma_j^2 u^2(T)$. In the EXAFS spectra, DWF refers to correlated averages over the relative displacement of $\sigma^2(T)$ for a pair of absorber and backscatter atoms. While neutron diffraction refers to the Mean Square Displacement (MSD) $u^2(T)$ of a given atom. The functions $\sigma^2(T)$ and $u^2(T)$ are closely related to one another, and from them, the Displacement-Displacement Correlation Function $C_R(T)$ can be deduced to describe the correlation effects in the vibration of atoms. The DWF has an essential role in the determination of crystal structures as well as thermal quantities in the EXAFS spectra.Have been many studies to derive the procedures for the calculation and analysis of $\sigma^2(T)$ [5], [13], [14], and $u^2(T)$ [1], [12]. However, correlation effects for intermetallic alloys have not mentioned by many studies.

In this work, correlation effects were analyzed and are described by the $C_R(T)$ function based on DWF in EXAFS. Analytical expressions were determined for the $\sigma^2(T)$ function based on the Anharmonic Correlated Debye Model (ACDM) and for the $u^2(T)$ function based on the Anharmonic Debye Model (ADM), ratios of $\sigma^2(T)$, $u^2(T)$ and $C_R(T)$ were considered. The effects of multi-particle systems were taken into account in the present one-dimensional model by a simple measure based on the derived anharmonic effective potentials that include the interactions of absorber and backscatter atoms with their nearest neighbours. Single-pair interactions of atoms are described by the Morse potential. The studies were analyzed the difference between the $\sigma^2(T)$ obtained from the ACDM and $u^2(T)$ from the ADM. Simultaneously, the analytical expressions were created for face-centred-cubic (fcc) crystal and its alloys.The numerical results for application to copper (Cu), silver (Ag) crystals and CuAg72, CuAg50 alloys. The expression CuAg72 refers to an alloy with 72% of Cu and 28% of Ag ratio, and CuAg50 refers to an alloy with Cu:Ag in a 50:50 ratio (or 1:1 ratio).These materials have been of interest to the authors in a few recent studies [3], [4]. The results obtained by the present theory agree well with experimental values [6], [10], [11] and other studies [1], [4], [9].

2. Formalism

In the Eq. (1), the quantity $\sigma^2(T)$ is defined while taking the exponential averages $exp(2i\kappa r_j)$ in the form [2]

$$\Big\langle exp(2i\kappa r_j)\Big\rangle \rightarrow \Big\langle exp(2i\kappa\Gamma_j)\Big\rangle = \Big\langle exp(-2\kappa^2\Gamma_j^2)\Big\rangle. \tag{2}$$

In Eq.(2), $\Gamma_j = \hat{\Re}_j^0.(u_j - u_0)$ where $\hat{\Re}_j^0$ is a unit vector for atom j at equilibrium, u_j is a displacement vector of atom j, and u_0 is the displacement vector of the absorber atom located at the coordinate origin. For the harmonic approximation oscillation,

$$\sigma_j^2 = \Big\langle \Gamma_j^2 \Big\rangle. \tag{3}$$

Substitute $\Gamma_j = \hat{\Re}_j^0.(u_j - u_0)$ into expression (3), $\sigma^2(T)$ has the form:

$$\sigma_j^2(T) = \Big\langle \Big[\hat{\Re}_j(u_j - u_0)\Big]^2 \Big\rangle = \Big\langle (u_j.\hat{\Re}_j)^2 \Big\rangle + \Big\langle (u_0.\hat{\Re}_j)^2 \Big\rangle - 2\Big\langle (u_j.\hat{\Re}_j)(u_0.\hat{\Re}_j) \Big\rangle. \tag{4}$$

With $u_0 = u_j$, the $u^2(T)$ as:

$$u_j^2(T) = \Big\langle (u_j.\hat{\Re}_j)^2 \Big\rangle = \Big\langle (u_0.\hat{\Re}_j)^2 \Big\rangle, \tag{5}$$

and the correlated function $C_R(T)$:

$$C_R(T) = 2\Big\langle (u_0.\hat{\Re}_j).(u_j.\hat{\Re}_j) \Big\rangle. \tag{6}$$

From expressions (4,5,6), the relation expression between of the quantities can be deduced:

$$\sigma_j^2(T) = 2u_j^2(T) - C_R(T). \tag{7}$$

To determine the quantities $\sigma^2(T)$, $u^2(T)$, and $C_R(T)$ with an anharmonic effect, we need to determine the effective spring force constants (force constants - FC) of atomic pairs in a cluster of the nearest atoms. The determination of FCs is based on the effective anharmonic potential

as a function along the direction of the displacement x. According to ACDM, the anharmonic potential has the following form [8], [10]:

$$U^A_{eff}(x) \approx \frac{1}{2}k^A_{eff}x^2 + k^A_{3eff}x^3, \tag{8}$$

and in the ADM has the form;

$$U^A_{eff}(x) \approx \frac{1}{2}k^D_{eff}x^2 + k^D_{3eff}x^3, \tag{9}$$

here k^A_{eff}, and k^D_{eff} are FCs, k^A_{3eff} and k^D_{3eff} are cubic parameters that cause asymmetry of the interaction potential due to anharmonicity, x is the lattice thermal expansion r, r_0 are the distance between two atoms at temperature T, and its value at the equilibrium position, respectively. The difference between the FCs and cubic parameters (PCs) lead to the difference between $U^A_{eff}(x)$ and $U^D_{eff}(x)$ potentials in the Eqs. ()8, 9).
The values of the FCs and the PCs can be obtained when effective potentials are determined. Assume M_1 is the mass of the absorbing atom, and the scattering atomic mass is M_2, and take on that the atomic mass is in the centre of the pair of absorbing and scattering atoms.

In the ACDM, the potential $U^A_{eff}(x)$ will take the form;

$$U^A_{eff}(x) = U(x) + \sum_{i\neq j} U\Big(\frac{\mu}{M_i}x\hat{\Re}_{12}.\hat{\Re}_{ij}\Big), \tag{10}$$

where $U(x)$ represents an interaction potential between absorber and backscatter atoms, the sum of i over absorber ($i = 1$) and backscatter ($i = 2$) atoms and the sum of j over their nearest neighbours in a cluster of atoms describe the lattice contributions to pair interactions and depend on the crystal structure type. $\hat{\Re}$ is the unit vector, $\mu = (M_1M_2)/(M_1 + M_2)$ is the reduced mass. For simplicity, we assume $M_1 = M_2 = M$ and $\mu = M/2$. For fcc crystals, the potential $U^A_{eff}(x)$ as:

$$U^A_{eff}(x) = U(x) + 2U\Big(-\frac{x}{2}\Big) + 8U\Big(-\frac{x}{4}\Big) + 8U\Big(\frac{x}{4}\Big). \tag{11}$$

Similarly, according to the ADM, the $U^D_{eff}(x)$ potential with an expression of the single-particle effective potential, and when only the influence of N neighbour atoms is taken into account, the $U^D_{eff}(x)$ potential can be written as

$$U^D_{eff}(x) = \sum_{j=1}^{N} U\Big(x\hat{\Re}^0.\hat{\Re}_j\Big), \tag{12}$$

where $\hat{\Re}_j$ is the jth atom unit vector from the equilibrium site, for fcc crystals:

$$U^A_{eff}(x) = U(x) + U(-x) + 4U\Big(\frac{x}{2}\Big) + 4U\Big(-\frac{x}{2}\Big). \tag{13}$$

The use of the effective potentials in the above equations changed the complex three-dimensional problem for multi-particle effects into a more straightforward one-dimensional problem.
Expansion the Morse potential to the third-order around a minimum point:

$$U_(x) = G\Big(e^{-2\varphi x} - 2e^{-2\varphi x}\Big) \approx G\Big(-1 + \varphi^2x^2 - \varphi^3x^3 + ...\Big), \tag{14}$$

where ϕ is the width of the potential, and G is the dissociation energy. For intermetallic alloys AB, if the two-component symbols of alloys follow the indexes 1 and 2, we have φ_{12} and G_{12}. Their values are calculated as a percentage of alloy doping [4].

According to the ACDM, FCs as:

$$k^A_{eff} = 5G_{12}\varphi^2_{12}, \quad k^A_{3eff} = -\frac{3}{4}G_{12}\varphi^3_{12}, \tag{15}$$

and the ADM as:

$$k^D_{eff} = 8G_{12}\varphi^2_{12}, \quad k^A_{3eff} = -G_{12}\varphi^3_{12}. \tag{16}$$

Derivation the expressions (4, 5, 6). Describe the system in the Debye model involving all frequencies up to the Debye frequency, each of which corresponds to a wave with a frequency $\omega(q)$ and different wavenumbers. Based on ACDM, $\sigma^2(T)$ has the form;

$$\sigma^2(T) = \frac{\hbar c}{2\pi k^A_{eff}} \int_0^{\frac{\pi}{c}} \omega_A(q) \frac{1 + z_A(q)}{1 - z_A(q)} dq, \tag{17}$$

$$z_A(q) = e^{\beta\hbar\omega_D(q)}, \quad \omega_D(q) = 2\sqrt{\frac{2k^D_{eff}}{M}}|(\sin qc/2)|, \quad \beta = \frac{1}{k_b T}. \tag{18}$$

Substitute from Eq. (5) into Eqs. (17), (18), it has the following form $\sigma^2(T)$:

$$\sigma^2(T) = \frac{\hbar c}{10\pi G_{12}\varphi^2_{12}} \int_0^{\frac{\pi}{c}} \omega_A(q) \frac{1 + z_A(q)}{1 - z_A(q)} dq, \tag{19}$$

$$z_A(q) = e^{\beta\hbar\omega_A(q)}, \quad \omega_A(q) = 2\sqrt{\frac{10G_{12}\varphi^2_{12}}{M}}|(\sin qc/2)|, \quad |q| \leq \frac{\pi}{c}. \tag{20}$$

Similarly, for ADM, the $u^2(T)$ have been determined as

$$u^2(T) = \frac{\hbar c}{2\pi k^D_{eff}} \int_0^{\frac{\pi}{c}} \omega_D(q) \frac{1 + z_D(q)}{1 - z_D(q)} dq, \tag{21}$$

$$z_D(q) = e^{\beta\hbar\omega_D(q)}, \quad \omega_D(q) = 2\sqrt{\frac{2k^D_{eff}}{M}}|(\sin qc/2)|, \tag{22}$$

from Eq. (16) into Eqs. (21, 22), will obtain

$$u^2(T) = \frac{\hbar c}{16\pi G_{12}\varphi_{12}} \int_0^{\frac{\pi}{c}} \omega_D(q) \frac{1 + z_D(q)}{1 - z_D(q)} dq, \tag{23}$$

$$z_D(q) = e^{\beta\hbar\omega_D(q)}, \quad \omega_D(q) = 2\sqrt{\frac{8G_{12}\varphi^2_{12}}{M}}|(\sin qc/2)|, \quad |q| \leq \frac{\pi}{c}, \tag{24}$$

where c is the lattice constant, q is the phonon wavenumber, and M is the mass of composite atoms. From Eqs. (19, 20, 23, 24), and (7), we have the correlated function $C_R(T)$:

$$C_R(T) = \frac{\hbar c}{2\pi}\Big\{\frac{1}{k^D_{eff}}\int_0^{\frac{\pi}{c}}\omega_D(q)\frac{1+z_D(q)}{1-z_D(q)}dq - \frac{1}{k^A_{eff}}\int_0^{\frac{\pi}{c}}\omega_A(q)\frac{1+z_A(q)}{1-z_A(q)}dq\Big\}, \quad |q| \le \frac{\pi}{c}. \tag{25}$$

Substitute Morse potential parameters for fcc crystals into Eq.(25), will obtain the correlation function

$$C_R(T) = \frac{\hbar c}{2G_{12}\varphi_{12}}\Big\{\frac{1}{4}\int_0^{\frac{\pi}{c}}\omega_D(q)\frac{1+z_D(q)}{1-z_D(q)}dq - \frac{1}{5}\int_0^{\frac{\pi}{c}}\omega_A(q)\frac{1+z_A(q)}{1-z_A(q)}dq\Big\}, \quad |q| \le \frac{\pi}{c}. \tag{26}$$

3. Numerical results and discussion

Using the Eqs. (19-26) to calculate for Cu, Ag, CuAg72, and CuAg50 crystals. The results of the theoretical calculation of the Morse potential parameter and the experimental Morse parameters [10] listed in Table 1, and the FCs listed in Table 2. The data in the tables show the agreement of the theoretical calculations with experimental measure values and other studies [6], [10], [11], [14], [15]. Substituting the parameters in Tables 1 and 2 into Eqs. (19), (23), (26), we will get the $\sigma^2(T)$, $u^2(T)$, and $C_R(T)$ for Cu crystals and CuAg72 CuAg50 alloys.

Quantities/ Crystals	$G_{12}(eV)$ (Present)	$G_{12}(eV)$ (Expt.)	$\varphi_{12}(\mathring{A}^{-1})$ Present)	$\varphi_{12}(\mathring{A}^{-1})$ (Expt.)
Ag-Ag	0.3429	0.3528	1.3588	1.4072
Cu-Cu	0.3323	0.3253	1.3690	1.3535
CuAg72	0.3381	-	1.3634	-
CuAg50	0.3376	-	1.3638	-

Table 1: Morse potential parameters G_{12} and φ_{12}.

There is a significant difference between the correlation oscillation model and the single-particle anharmonic oscillation model. The reason for this difference is the determination of the number and mass of atoms oscillating in two models. For the correlation oscillation model, the quantity and mass of particles are only half those of the single-particle anharmonic oscillator. In the correlated oscillation model, a crystal will act as quasi-atoms. That means that the mass reduced to equal only half of the composite atomic mass, and the number of atoms is only half the number of atoms for a single-particle anharmonic vibration model.

Figure 1 shows the temperature dependence of $\sigma^2(T)$ (Fig. 1a) and $u^2(T)$ (Fig. 1b) for Cu, Ag and CuAg72 and CuAg50 crystals. They show linear proportional to the temperature T at high temperatures. At the same temperature, the values of $\sigma^2(T)$ are greater than the values

Quantities/ Crystals	$k^A_{eff}(eVA^{-2})$ (Present)	$k^A_{eff}(eVA^{-2})$ (Present)	$k^D_{eff}(eVA^{-2})$ (Present)	$k^D_{eff}(eVA^{-2})$ (Expt.)
Cu-Cu	3.1655	3.4931	5.5889	5.7520
Ag-Ag	3.1139	2.9797	5.3254	-
CuAg72	3.1423	-	5.0278	-
CuAg50	3.1396	-	5.0234	-

Quantities/ Crystals	$k^A_{3eff}(eVA^{-3})$ (Present)	$k^A_{3eff}(eVA^{-3})$ (Present)	$k^D_{3eff}(eVA^{-3})$ (Present)	$k^D_{3eff}(eVA^{-3})$ (Expt.)
Cu-Cu	1.0753	1.2289	1.0889	0.9831
Ag-Ag	1.0657	1.0083	1.1354	-
CuAg72	0.6814	-	2.6874	-
CuAg50	0.6423	-	0.8569	-

Table 2: Effective spring force constants and cubic parameters.

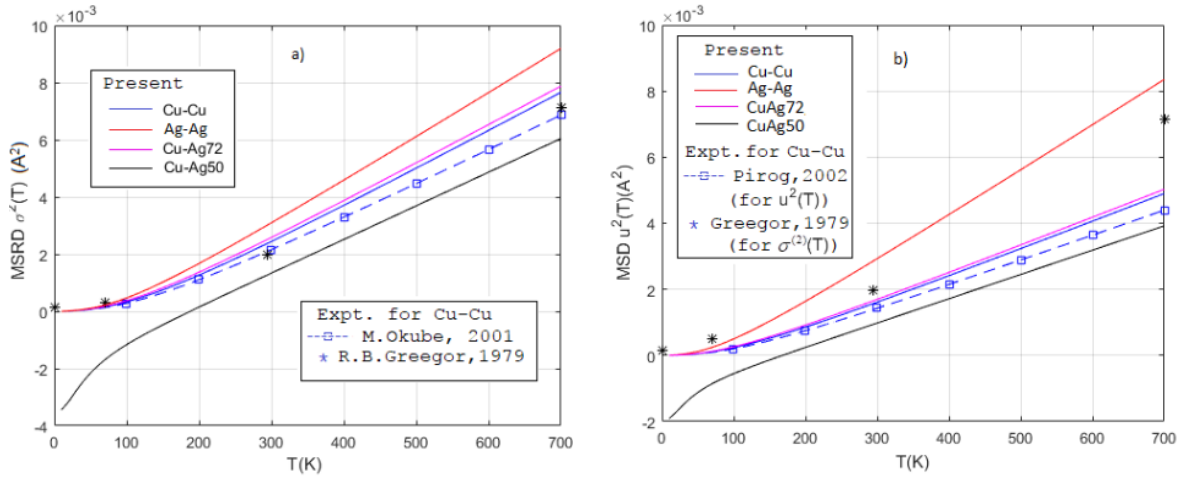

Figure 1. The temperature dependence of mean square relative displacement (a) and mean square relative displacement (b) for Cu,Ag, CuAg72 and CuAg50 crystal alloys

of $\sigma^2(T)$, which is evident in Fig. 1b. The experimental values of $\sigma^2(T)$ (symbol points *) are higher with the experimental curves of $u^2(T)$ [6].

Figure 2 illustrates the dependence of the $C_R(T)$ on temperature for Cu, Ag crystal and CuAg72 and CuAg50 alloys. Similar to the graphs depicting the dependence on temperature of $\sigma^2(T)$ (Fig. 1a) and $u^2(T)$ (Fig. 1b), they are all linearly proportional to the temperature T at high temperatures, the classical limit is applicable. At low temperatures, the curves for Cu, Ag and CuAg72 contain zero-point energy contributions - a quantum effect. The calculated results of $\sigma^2(T)$, $u^2(T)$ and $C_R(T)$ for the Cu, Ag crystal fitting well with the experimental values [6], [10], [15]. Thus, it is possible to deduce that the calculation results of the present method for CuAg72, CuAg50 are reasonable. Moreover, the values of $\sigma^2(T)$ are greater than those of $u^2(T)$, making the damping coefficients in EXAFS of the correlation oscillation model larger than those of single-particle anharmonic oscillation models.

Figure 3 shows the temperature dependence of the correlated ratios $C_R(T).u^2(T)/\sigma^2(T)$, the graph illustrates linearly proportional to the temperature T at high temperatures and suitable the curve line inferred from the empirical data (dashed line blue, Pirog, 2002). Opposite, Figure 4 illustrates the temperature dependence of the correlated ratios $\sigma^2(T)/C_R(T).u^2(T)$, the values decreased very quickly at low temperatures, unchanged at high temperatures reflected the correlation effect between these quantities in the classical theories.

Note that, have an attractive characteristic in all figures is the curves of CuAg72 and CuAg50 inter-metallic alloys. For the CuAg72 alloy, the shape of the curve is similar to the curvature

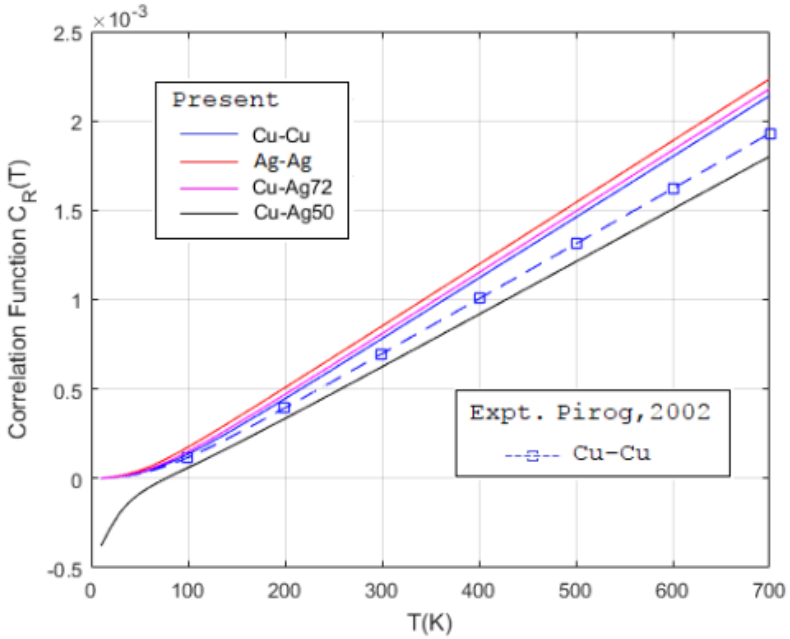

Figure 2. Temperature dependence of the correlation function $C_R(T)$ for Cu,Ag, CuAg72 and CuAg50 crystals

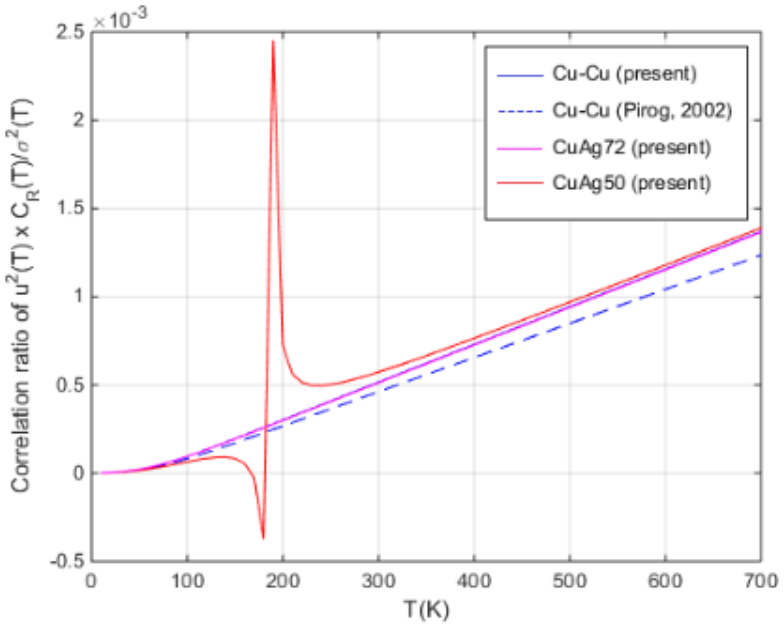

Figure 3. Correlation ratios of $u^2(T).C_R(T)/\sigma^2(T)$ for Cu,Ag, CuAg72 and CuAg50

of pure Cu, Ag crystals, meaning that the structure of the CuAg72 alloy is not broken still fcc structure type. However, for the CuAg50 alloy (black lines in Figs. 1, 2 and red lines in Figs. 3, 4), the curves have an abnormal shape, does not zero-point energy, and does not follow the rules like of Cu, Ag and CuAg72 at low temperatures (in the range from 140 K to 200 K, more clearly in the Figs. 3, 4a, 4b). At higher temperatures 200 K, the curve gradually returns to forms like of Cu, Ag and CuAg72 crystals. It is speculated that for the CuAg alloy at a ratio of

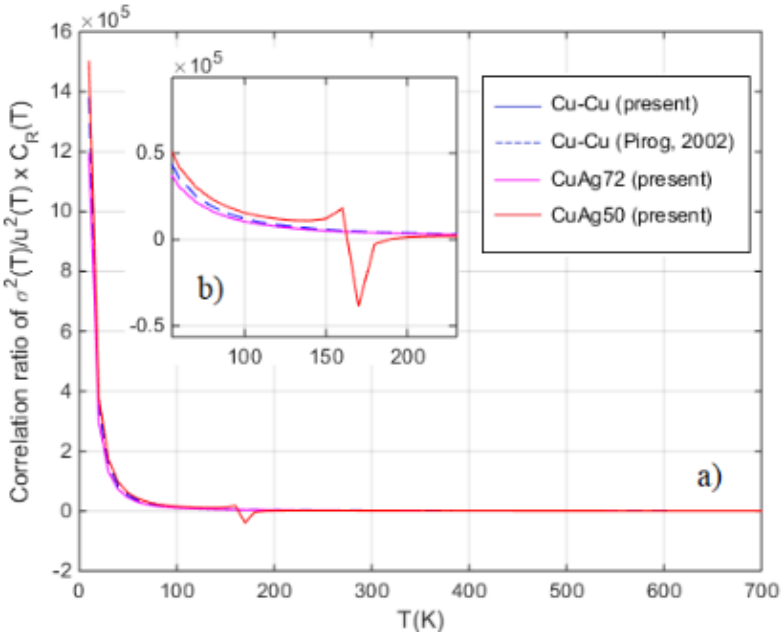

Figure 4. Correlation ratios of $\sigma^2(T)/C_R(T).u^2(T)$ for Cu,Ag, CuAg72 and CuAg50

50:50 (or 1:1 ratio), the atoms are no longer closely linked to each other in the style of the fcc lattice at low temperatures (meaning that no Cu-Ag alloy material exists in this ratio, Cu:Ag = 50:50). As the temperature increases, the correlation between the atoms changes until the temperature reaches a certain value (over 200 K). The fcc lattice order slowly recovers, and the graph curve of CuAg50 returns like to the Cu, Ag and CuAg72. It is entirely reasonable with studies done with other models and theories, as well as experiments with the Cu-Ag alloy at the percentage ratio of 1:1 (CuAg50) [4], [9].

4. Conclusions

In this work, the correlation effects of the displacement correlation function, mean square relative displacement, and the mean square displacement in EXAFS spectra and their ratios were deduced and analyzed. The theory was applied to Cu, Ag, CuAg72, CuAg50 crystals and alloys. The analytical expressions of $C_R(T)$, $\sigma^2(T)$, and $u^2(T)$ were inferred based on Debye models. The advantage of these models is based on the use of anharmonic effective potentials, which take the contributions of all the nearest neighbouring atoms. The difference of the effective spring force constant and the difference in the number and mass of vibrating atoms in these models causes a difference in the thermodynamic properties of the crystals.

The values of $\sigma^2(T)$, $u^2(T)$, and $C_R(T)$ are all linearly proportional to the temperature T at high temperatures, and the classical limit is applicable. At low temperatures, they contain zero-point energy contributions, a quantum effect. The correlated ratios $C_R(T).u^2(T)/\sigma^2(T)$ linearly proportional to the temperature T at high temperatures agree well for the curve line inferred from the empirical data (dashed line blue, Pirog, 2002). Opposite, the correlated ratios $\sigma^2(T)/C_R(T).u^2(T)$ are constant at high temperatures, correctly reflected the correlation between these quantities in the EXAFS classical theories.

The crystal lattice of the CuAg50 alloy showed an abnormal disorder at rank 140K-180K temperatures. We speculate that Cu and Ag atoms no longer closely had linked lattice structures the fcc structure type, that means, CuAg alloy material with a ratio of 50:50 (or 1:1 ratio), does not exist at temperatures approximation from 140K to 200K. This result discovered by

Kraut and Stern (2000) as well as other theoretical studies by Nguyen, Vu (2019), and Nguyen (2020). These anomalies may give rise to many new interesting in-depth studies for researchers specializing in materials science.

The good agreement between the calculation results of the present study and the values obtained from experiments and calculations according to other models prove the effectiveness of the present theory in EXAFS spectrum data analysis.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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