Physica B: Condensed Matter 552 (2019) 1–5

Contents lists available at ScienceDirect

Physica B: Condensed Matter

journal homepage: www.elsevier.com/locate/physb

Dependence of cumulants and thermodynamic parameters on temperature and doping ratio in extended X-ray absorption fine structure spectra of cubic crystals

Nguyen Ba Duc*, Vu Quang Tho

Department of Physics, Tan Trao University, Tuyen Quang, Viet Nam

ARTICLE INFO

Keywords:
Anharmonic
EXAFS
Cumulants
Thermodynamic
Doping ratio

ABSTRACT

The thermodynamic properties and anharmonic perturbation factor of orderly doped crystals are described in terms of the cumulants in extended X-ray absorption fine structure (EXAFS) spectra. The thermodynamic parameters and cumulants are studied based on the anharmonic correlated Einstein model. We derive analytical expressions for the dispersion relation, the correlated frequency and Einstein temperature, and the EXAFS cumulants. Parameters of the Morse potential, thermal expansion coefficient due to effect of anharmonicity, anharmonic factor, the EXAFS phase including the anharmonic effects depend on doping ratio of cubic-structure crystals are considered. The derived anharmonic effective potential includes the contributions of all the nearest neighbors of the absorbing and scattering atoms to account for three-dimensional interactions and the parameters of the Morse potential to describe single-pair atomic interactions. Numerical results for face-centered cubic (fcc) crystals of copper (Cu—Cu) and silver (Ag—Ag) and their compound Ag—Cu agree reasonably with experiments and other theories.

1. Introduction

To study how the cumulants, thermal parameters, and thermodynamic properties of lattice crystals of a substance depend on the temperature and their doping ratio (DR), in previous studies we have used extended X-ray absorption fine structure (EXAFS) spectra, an approach that has developed into a powerful probe of the atomic structures and thermal effects of substances [1,3,4,6–11]. The functions of EXAFS spectra provide information about the atomic number of each shell, and their Fourier magnitudes provide information about the radius of this atomic shell [1,4,8,9]. The thermodynamic parameters and the EXAFS cumulants up to third order have been derived for pure cubic crystals by using the anharmonic correlated Einstein model (ACEM) in EXAFS theory [7,9]. However, the thermodynamic parameters, cumulants, anharmonic perturbation factor, and thermal expansion coefficient for doped face-centered cubic (fcc) crystals, such as crystals of copper (Cu) doped with silver (Ag) (Ag—Cu), are yet to be determined.

In the present study, we use the anharmonic effective Einstein potential in EXAFS theory [7] to formulate thermodynamic parameters such as the effective force constant, anharmonic factor, thermal expansion coefficient, cumulant expressions, and some other parameters such as the correlated Einstein frequency and correlated Einstein temperature that are contained in the EXAFS spectra. In this study, the Ag—Cu doped crystals contain Ag atoms (referred to as the substitute atoms) and Cu atoms (referred to as the host atoms). Numerical calculations have been conducted for Ag—Cu doped crystals to show the thermodynamic effects and how they depend on the DR and temperature of fcc crystals. The calculated results are in good agreement with those of other studies [2,5,7,8].

2. Formalism

An anharmonic EXAFS spectrum is often expressed as [4,7].

$$\chi(k)=\frac{S_0^2N}{kR^2}F(k)\exp\left(-\frac{2R}{\lambda(k)}\right)\mathrm{Im}\left(e^{i\Phi(k)}\exp\left(2ikr_0+\sum_n\frac{(2ik)^n}{n!}\sigma^{(n)}(T)\right)\right), \tag{1}$$

where S_0^2 is the intrinsic loss factor due to many electron effects, N is the atomic number of a shell, $F(k)$ is the atomic backscattering amplitude, $\Phi(k)$ is the total phase shift of the photoelectron, k and λ are the wave number and mean free path of the photoelectron, respectively, and $\sigma^{(n)}$ ($n = 1, 2, 3, 4\ldots$) are the cumulants and describe the asymmetric components of the interactive potential. The latter are due to the

---

* Corresponding author.
E-mail addresses: ducnb@daihoctantrao.edu.vn, duc.xafs@gmail.com (N.B. Duc).

https://doi.org/10.1016/j.physb.2018.09.038
Received 31 August 2018; Accepted 25 September 2018

thermal average of the function e^{-2ikr}, in which the asymmetric terms are expanded as a Taylor series around $R = <r>$, where r is the instantaneous bond length between absorbing and scattering atoms at temperature T.

In the ACEM, [7,8] the effective interaction between absorbing and scattering atoms with contributions from the atomic neighbors is characterized by an effective potential. To determine the Debye–Waller factor (DWF) in terms of the cumulants, it is necessary to specify the interatomic potential and force constant. Consider a high-order expanded anharmonic interatomic effective potential expanded up to fourth order, namely

$$U(x) \approx \frac{1}{2}k_{eff}x^2 + k_{3eff}x^3 + k_{4eff}x^4 + \ldots \tag{2}$$

with net deviation $x = r - r_0$, where r is the spontaneous bond length between absorbing and backscattering atoms and r_0 is its equilibrium value. In Eq. (2), k_{eff} is an effective spring constant that includes the total contribution of the neighboring atoms, and k_{3eff} and k_{4eff} are effective anharmonicity parameters that specify the asymmetry of the anharmonic effective potential.

The effective potential given by Eq. (2) is defined based on an assumption in the orderly center-of-mass frame of a single-bond pair of an absorber and a bacskcatterer [7,8]. For monatomic crystals, the masses of the absorber and backscatter are the same, so the effective potential is given by

$$U_E(x) = U(x) + \sum_{i=0,1}\sum_{j\neq i} U\left(\frac{\mu}{M_i}x\,\widehat{\mathrm{R}}_{01}.\widehat{\mathrm{R}}_{\mathrm{ij}}\right) = U(x) + 2U\left(-\frac{x}{2}\right) + 8U\left(-\frac{x}{4}\right) + 8U\left(\frac{x}{4}\right), \tag{3}$$

where the first term on the right-hand side, namely $U(x)$, concerns only absorber and backscatter atoms. The sums extend over their nearest neighbors, and the second equality is for the fcc structure of Cu orderly doped with Ag. Therefore, this effective pair potential describes not only the pair interaction of the absorber and backscatter atoms themselves but also how their near-neighbors atoms affect such interaction. It is the difference between our effective potential and the single-pair potential [6] and single-bond potential, [1] which concern only each pair of immediate neighboring atoms (i.e., only $U(x)$) without the remaining terms on the right-hand side of Eq. (3). In Eq. (3), $\widehat{\mathrm{R}}$ is the unit bond-length vector, μ is the reduced atomic mass, and the summation over i and j is the contribution of the cluster of nearest atoms. The atomic vibration is calculated based on a quantum statistical procedure with an approximate quasi-harmonic vibration, in which the Hamiltonian of the system is written as a harmonic term with respect to the equilibrium at a given temperature plus an anharmonic perturbation:

$$H = \frac{P^2}{2\mu} + U_E(\chi) = H_0 + U_E(a) + \delta U_E(y), \quad H_0 = \frac{P^2}{2\mu} + \frac{1}{2}k_{eff}y^2, \tag{4}$$

with $y = x - a$, $a(T) = \langle x\rangle$, and $\langle y\rangle = 0$, where a is the net thermal expansion and y is the deviation from the equilibrium value of x at absolute temperature T. The potential interaction between each pair of atoms in the single bond can be expressed by the anharmonic Morse potential for cubic crystals. Expanding to fourth order, we have

$$U_E(x) = D(e^{-2\alpha x} - 2e^{-\alpha x}) \approx D\left(-1 + \alpha^2x^2 - \alpha^3x^3 + \frac{7}{12}\alpha^4x^4\ldots\right), \tag{5}$$

where D is the dissociation energy by $U(r_0) = -D$ and α describes the width of the potential. For orderly doped crystals, we assign the host atom the indicator 1 and the substitute atom the indicator 2. Then we have the Morse potential expressed by Eq. (5) for the case of doped material, namely

$$U_E(x) = D_{12}\left(-1 + \alpha_{12}^2x^2 - \alpha_{12}^3x^3 + \frac{7}{12}\alpha_{12}^4x^4\ldots\right). \tag{6}$$

For simplicity, we approximate the parameters of the Morse potential in Eq. (6) at a certain temperature by the following arithmetic averages:

$$D_{12} = \frac{D_1 + D_2}{2}, \quad \alpha_{12}^2 = \frac{D_1\alpha_1^2 + D_2\alpha_2^2}{D_1 + D_2}, \quad \alpha_{12}^3 = \frac{D_1\alpha_1^3 + D_2\alpha_2^3}{D_1 + D_2}. \tag{7}$$

From Eqs. (3) and (6), we obtain the Einstein potential of the effective interaction as

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

We calculate $(\widehat{\mathrm{R}}_{01}.\widehat{\mathrm{R}}_{\mathrm{ij}})$ in Eq. (3) for lattice fcc crystals, substitute Eq. (6) with $x = y + a$ into Eq. (3), and use Eq. (8) to calculate the sums in the second term of Eq. (3) with the reduced mass μ of the doped metals. By comparing the results to Eq. (4), we determine the coefficients k_{eff} and k_{3eff} of the anharmonic effective potential in terms of the parameters of the Morse potential, namely

$$k_{eff} = 5D_{12}\alpha_{12}^2, \; k_{3eff} = \frac{5D_{12}\alpha_{12}^3}{4}. \tag{9}$$

To derive analytical formulas for the cumulants of the fcc crystals, we use perturbation theory.[15] The atomic vibration is quantized as phonons. Considering the phonon–phonon interactions to account for anharmonicity effects, we obtain the cumulants up to third order:

$$\sigma^{(1)} = \langle x\rangle = \frac{3\hbar}{40D_{12}\alpha_{12}}\sqrt{\frac{k_{eff}}{\mu_{12}}}\frac{\left(1 + exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{\mu_{12}}}\right)\right)}{\left(1 - exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{\mu_{12}}}\right)\right)}, \tag{10}$$

$$\sigma^{(2)} = \langle x^2\rangle - \langle x\rangle^2 \approx \langle x^2\rangle = \frac{\hbar}{10D_{12}\alpha_{12}^2}\sqrt{\frac{k_{eff}}{\mu_{12}}}\frac{\left(1 + \exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{\mu_{12}}}\right)\right)}{\left(1 - \exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{\mu_{12}}}\right)\right)}, \tag{11}$$

$$\begin{aligned}\sigma^{(3)} &= \langle x^3\rangle - 3\langle x^2\rangle\langle x\rangle + 2\langle x\rangle^2 \\ &= \frac{3\hbar^2\frac{k_{eff}}{\mu_{12}}}{200D_{12}^2\alpha_{12}^3}\frac{\left(1 + 10\exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{\mu_{12}}}\right) + \left(\exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{\mu_{12}}}\right)\right)^2\right)}{\left(1 - \exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{\mu_{12}}}\right)\right)^2}.\end{aligned} \tag{12}$$

In Eqs. (10)–(12), T is the absolute temperature and k_B is the Boltzmann constant. Equations (10)–(12) describe how the cumulants depend on the reduced mass μ_{12} of the doped metals and the absolute temperature T. If we consider that, at a certain temperature, the reduced mass μ_{12} is proportional to the number of atoms, meaning that the cumulants depend on the DR of the materials. We express the reduced atomic mass being proportional to the number n of atoms of the Cu and Ag metals as

$$\mu_{12} = 108 - 44.5n, \quad \mu_1 = 63.5n, \quad \mu_2 = 108(1 - n). \tag{13}$$

Substituting Eq. (13) into Eqs. (10)–(12), we have the dependence of the cumulants on the number of atoms n:

$$\sigma^{(1)} = a = \frac{3\hbar}{40D_{12}\alpha_{12}}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\frac{\left(1 + exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)}{\left(1 - exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)}, \tag{14}$$

$$\sigma^{(2)} = \frac{\hbar}{10D_{12}\alpha_{12}^2}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\frac{\left(1 + \exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)}{\left(1 - \exp\left(-\frac{\hbar}{k_BT}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)}, \tag{15}$$

$$\sigma^{(3)} = \frac{3\hbar^2 \frac{k_{eff}}{108 - 44.5n}}{200 D_{12}^2 \alpha_{12}^3} \frac{\left(1 + 10\exp\left(-\frac{\hbar}{k_B T}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right) + \left(\exp\left(-\frac{\hbar}{k_B T}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)^2\right)}{\left(1 - \exp\left(-\frac{\hbar}{k_B T}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)^2}. \tag{16}$$

Next, we have that the general volumetric coefficient of thermal expansion is given by

$$\alpha_T = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P, \tag{17}$$

where V is the volume corresponding to the change of absolute temperature T under pressure P. From the equation of state of the thermal system, we have

$$\alpha_T = \frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T \left(\frac{\partial P}{\partial T}\right)_V, \tag{18}$$

where $V\left(\frac{\partial P}{\partial V}\right)_T$ is the elastic modulus that determines the change of volume due to pressure interaction. We ignore links between the atomic vibrations and assume the Helmholtz free energy to be of the form $F = U + \sum_q F_q$, and U is the total potential energy and F_q is the free energy and arises from lattice vibrations with wave vector q. Then the pressure depends on the volume according to

$$P = -\left(\frac{\partial F}{\partial V}\right)_T = -\frac{dU}{dV} - \sum_q \frac{dF_q}{dV} = -\frac{dU}{dV} - \sum_q \hbar \frac{\partial \omega_q}{\partial V}\left[\frac{1}{2} + \frac{1}{\exp\left(\frac{\hbar\omega_q}{k_B T} - 1\right)}\right]. \tag{19}$$

When anharmonic effects appear, the lattice system equilibrium at a new location and volume is expanded, so the important phenomenon associated with the anharmonic effect is the dependence of the net vibration frequency on volume. This dependence is described by the second term in Eq. (19).

To simplify, we assume that the volume dependence is the same at all net vibration frequencies and we consider the expansion in one dimension (linear thermal expansion), written in terms of the Grüneisen factor as

$$\omega \sim V^{-\gamma_G} \Rightarrow \gamma_G = -\frac{\partial(\ln \omega)}{\partial(\ln V)} = -\frac{\partial(\ln \omega)}{\partial a}\frac{\partial a}{\partial r}\frac{\partial r}{\partial(\ln V)}. \tag{20}$$

The factor γ_G characterizes the anharmonic effect with a net thermal coefficient:

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

Simultaneously, we have $a(T) - a(T_0) = da = \alpha_T r dT$.

From the above expression, we obtain the linear thermal expansion coefficient:

$$\alpha_T = \frac{1}{r}\frac{da}{dT}. \tag{21}$$

Substituting Eq. (14) into Eq. (21) and rearranging, we obtain the dependence of the linear thermal expansion coefficient on the absolute temperature T and the DR n of the metals:

$$\alpha_{T,n} = \frac{3k_B}{20 D_{12}\alpha_{12} r} \frac{exp\left(-\frac{\hbar}{k_B T}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\left[\ln\left(exp\left(-\frac{\hbar}{k_B T}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)\right]^2}{\left(1 - exp\left(-\frac{\hbar}{k_B T}\sqrt{\frac{k_{eff}}{108 - 44.5n}}\right)\right)^2}. \tag{22}$$

To consider the anharmonic contributions to the mean-square relative displacement (MSRD), we used an argument analogous to the one [3] for its change due to the temperature increase and obtain

$$\sigma^2(T) - \sigma^2(T_0) = [1 - \beta(T)][\sigma_H^2 - \sigma^2(T_0)], \quad \beta(T) = 2\gamma_G \frac{\Delta V}{V}. \tag{23}$$

Here, γ_G is the Grüneisen parameter, $\Delta V/V$ is the relative volume change due to thermal expansion, and T_0 is a very low temperature so that $\sigma^2(T_0)$ is a harmonic MSRD.

We calculate the relative thermal volume change $\Delta V/V$ using $R(T) = R + a(T)$ and the Grüneisen parameter in Eq. (20). By substituting the obtained results into Eq. (23), we derive the anharmonic factor as

$$\beta = \frac{9\eta k_B T}{16 D_{12}}\left[1 + \frac{3k_B T}{8 D_{12} R \alpha_{12}}\left(1 + \frac{3k_B T}{8 D_{12} R \alpha_{12}}\right)\right], \tag{24}$$

$$\eta = \frac{2\exp\left(-\frac{\theta_E}{T}\right)}{1 + \exp\left(-\frac{\theta_E}{T}\right)}.$$

This factor is proportional to the temperature and inversely proportional to the shell radius, thus reflecting a similar anharmonicity property obtained in experimental catalysis research [2] if R is considered as the particle radius. In the present work, we also consider how the anharmonic factor β depends on the atomic DR by an expression for the correlated Einstein temperature θ_E in Eq. (24):

$$\theta_E = \frac{\hbar\omega_E}{k_B}, \quad \omega_E = \sqrt{\frac{k_{eff}}{\mu_{12}}} = \sqrt{\frac{k_{eff}}{108 - 44.5n}}. \tag{25}$$

The anharmonic contribution Φ_A to the EXAFS phase at a given temperature is the difference between the total phase and that of the harmonic EXAFS. The EXAFS oscillation function Eq. (1) including anharmonic effects contains the DWF $e^{-w(kT)}$ that accounts for the effects of atomic thermal vibrations. Based on the analysis [9] of the cumulant expansion, we obtain

$$W\left(k, T\right) = 2ik\sigma^{(1)}(T) - 2k^2\sigma^2(T) - 4ik\sigma^2(T)\left(\frac{1}{R} - \frac{1}{\lambda(k)}\right) - \frac{4}{3}ik^3\sigma^{(3)}(T) + \frac{2}{3}\sigma^{(4)}(T)k^4 + ... \tag{26}$$

On the right-hand side of Eq. (26), the second and fifth terms contribute to the EXAFS amplitude. The only anharmonic contributions to the phase are the first and fourth terms and those to the MSRD in the third term. Therefore, from Eq. (26) we obtain the anharmonic contribution to the EXAFS phase as

$$\Phi_A\left(k, T\right) = 2k\left[\sigma^{(1)}(T) - 2\sigma_A^2(T)\left(\frac{1}{R} - \frac{1}{\lambda(k)}\right) - \frac{2}{3}k^2\sigma^{(3)}(T)\right]. \tag{27}$$

In Eq. (27), Φ_A depends not only on the absolute temperature T and the wave number k but also on the DR n of the metals.

3. Discussion and comparison of numerical results

The parameters of the Morse potential D and α for Ag–Ag, Cu–Cu crystals have been known [7], from Eq. (7), we calculate the parameters D_{12} and α_{12} as given in Table 1.

Substituting the thermodynamic parameters D_{12} and α_{12} from Table I into Eq. (9) with Boltzmann's constant $k_B = 8.617 \times 10^{-5}\text{eV}\text{Å}^{-1}$ and

Table 1
Parameter values of Morse potential for Ag, Cu, and Ag—Cu crystals.

Crystal	D_{12}(eV)	α_{12}(Å^{-1})
Ag—Ag	0.3323	1.3690
Cu—Cu	0.3429	1.3588
Ag—Cu	0.3376	1.3638

Table 2
Anharmonic effective parameter values.

Crystal	k_{eff} (eVA^{-2})	k_{3eff} (eVA^{-3})
Ag—Ag	3.1139	1.0657
Cu—Cu	3.1655	1.0753
Ag—Cu	3.1397	1.0705

Plank's constant $\hbar = 6.5822 \times 10^{-16} eV.s$, we calculate the values of the coefficients k_{eff} and k_{3eff} of the anharmonic effective potential in terms of the parameters of the Morse potential as given in Table 2.

Substituting the values of the thermodynamic parameters from Tables 1 and 2 into Eqs. (14)–(20), we obtain expressions for the cumulants $\sigma^{(n)}(n)$, the thermal expansion coefficient $\alpha(T, n)$, the anharmonic factor $\beta(T, n)$, and the contribution to the EXAFS phase $\Phi_A(T, n)$. The expressions depend on temperature and the metallic DR. Fig. 1 shows how our first three calculated cumulants depend on DR at a certain temperature (700 K) for the compound Ag—Cu. The graphs of $\sigma^{(1)}(T)$, $\sigma^{(2)}(T)$, and $\sigma^{(3)}(T)$ show that for DRs of zero to below 50% and from over 50%–100%, the cumulant values are proportional to the DR. However, there are breakpoints in the lines at the 50% point, meaning that we do not have ordered atoms at this ratio, which agrees with the findings of another study [4]. Thus in the present study, Ag—Cu alloys do not form an ordered phase at a molar composition of 1:1. From the temperature dependence of our calculated second cumulant or DWF for Ag—Cu, the latter became copper (Cu—Cu) at a ratio of 100% and agrees well with experimental value [7] (point $^{(*)}$ in Fig. 1).

Fig. 2 shows how our calculated thermal expansion coefficient $\alpha_{T,n}$ of Ag—Cu depends on temperature and DR. With the absolute temperature T, our $\alpha_{T,n}$ have the form of the specific heat C_V, thus reflecting the fundamental principle of solid state theory that the thermal expansion results from anharmonic effects and is proportional to the specific heat C_V [12]. Our calculated values of $\alpha_{T,n}$ approach the constant value α_T^0 at high temperatures and vanish exponentially with θ_E/T at low temperatures, which agrees with the findings of other research [11]. Our calculated thermal expansion coefficient $\alpha_{T,n}$ approaches being proportional to the DR from zero to below 50% and from over 50%–100%, but again there is a breakpoint at 50%, thereby agreeing with the evaluation by Kraut and Stern [5]. Fig. 3 shows how our calculated anharmonic contribution to the Ag—Cu, anharmonic factor $\beta(T, n)$ depends on temperature and DR. According to the graph, the anharmonic factor is proportional to the temperature and DR. It is approximately zero at low temperatures, thus reflecting an anharmonicity property that agrees well with those obtained previously [8]. Fig. 4 shows how our calculated anharmonic contribution to the EXAFS phase $\Phi_A(T, n)$ of Ag—Cu depends on temperature and DR for the first shell for single scattering. These contributions are especially large at high temperature and high DR and have breakpoints in the range of 50–70%. This result agrees with previous evaluation [5]. The anharmonic contribution $\Phi_A(T, n)$ to the EXAFS phase at a given temperature is the difference between the total phase and that of the harmonic EXAFS.

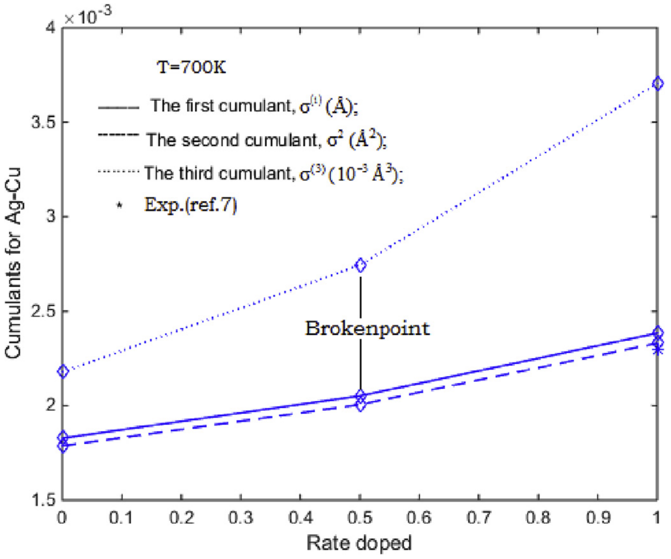

Fig. 1. Dependence of cumulants on doping ratio (DR).

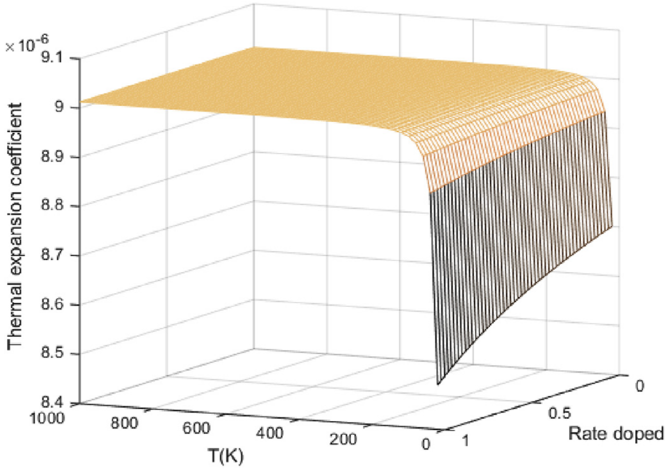

Fig. 2. Dependence of thermal expansion coefficient on temperature and DR.

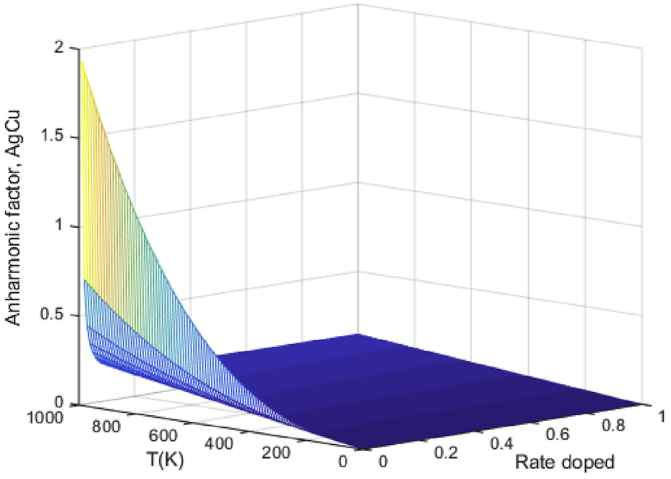

Fig. 3. Dependence of anharmonic factor on temperature and DR.

4. Conclusion

In this work, a new analytical theory for calculating and evaluating the thermodynamic properties of Ag—Cu fcc crystals has been developed based on quantum statistical theory with the effective anharmonic Einstein potential. The expressions for the thermodynamic parameters,

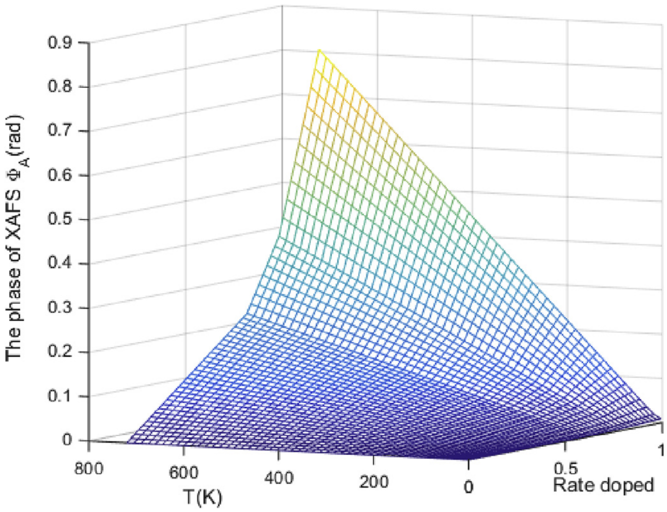

Fig. 4. Dependence of anharmonic EXAFS spectra phase on temperature and DR of Ag—Cu.

the effective force constant, the correlated Einstein frequency and temperature, the cumulants expanded up to third order, the thermal expansion coefficient, and the anharmonic factor in the anharmonic EXAFS spectra of Ag—Cu crystals agree with all the standard properties of these quantities. The expressions used for calculations for the orderly doped fcc crystals have similar forms to those for pure crystals. The graphs in Figs. 1–4 show dependence of thermodynamic parameters on temperature and DR of the fcc crystals, they reflect the properties of anharmonicity in EXAFS and agree well with those obtained in previous studies. The reasonable agreements between our calculated results with experimental and the other study for Ag—Cu indicate the efficiency of the present method in calculating and analyzing the thermodynamic properties of doped crystals based on ACEM in EXAFS theory.

References

[1] A.I. Frenkel, J.J. Rehr, Phys. Rev. B 48 (1993) 585.
[2] B.S. Clausen, L. Grabæk, H. Topsoe, L.B. Hansen, P. Stoltze, J.K. Norskǿv, O.H. Nielsen, J. Catal. 141 (1993) 368.
[3] B.N. Duc, N.V. Hung, H.D. Khoa, D.Q. Vuong, S.T. Tien, Adv. Mater. Sci. Eng. (2018) 32631709pp.
[4] N.V. Hung, N.B. Trung, B.N. Duc, J. Mater. Sci. Appl. 1 (3) (2015) 91–95.
[5] J.C. Kraut, W.B. Stern, J. Gold Bull. 33 (2) (2000) 52.
[6] J.M. Tranquada, R. Ingalls, Phys. Rev. B 28 (1997) 3520.
[7] N.V. Hung, N.B. Duc, R.R. Frahm, J. Phys. Soc. Jpn. 72 (5) (2002) 1254.
[8] N.V. Hung, Sy Tien Tong, Nguyen Ba Duc, Quoc Vuong Dinh, Mod. Phys. Lett. B 28 (21) (2014) 1450174.
[9] N.V. Hung, J.J. Rehr, Phys. Rev. B 56 (1997) 43.
[10] N.B. Duc, AASCIT Phys. 1 (1) (2015) 1.
[11] N.V. Hung, N.B. Duc, J. Commun. 10 (1) (2000) 15.
[12] N.B. Duc, H.K. Hieu, N.T. Binh, K.C. Nguyen, X-Ray Absorption Fine Structure: Basic and Applications, Sciences and Technics Publishing House, Hanoi, 2018.