Debye-Waller factor depend on temperature with the influence of doping ratio of the crystal structure metals in extended X-Ray absorption fine structure

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ABSTRACT: Effects of the doping ratio and temperature on the Debye-Waller factor (DWF) of metals was investigated using the extended X-ray absorption fine structure spectra. The numerical results agree reasonably with experiments and other theories.

Keywords: anharmonic; EXAFS; cumulants; thermodynamic; doping ratio.

1. INTRODUCTION: Extended X-ray absorption fine structure (EXAFS) spectra has developed into a powerful probe of atomic structures and the thermal effects of substances.[1 -12] The dependence of the DWF on the temperature was studied using this technique. However, the effect of the doping ratio (DR) and temperature on the thermodynamic parameters and DWF of the EXAFS for copper doped with zinc (Cu-Zn), copper doped with silver (Cu-Ag) is yet to be determined. In this study, we use anharmonic effective potential (AEP) from EXAFS theory[7,9] to formulate expressions of DWF of Cu-Ag, Cu-Zn doped crystals. The Ag, Zn atoms are referred to as the substitute atoms and the Cu atoms are referred to as the host atoms. The results of the calculations are in good agreement with experimental values and those of other studies.[2-11]

2. FORMALISM: The anharmonic EXAFS function $\chi(k)$, is often show in references [1,7]. In the anharmonic correlated Einstein model (ACEM),[7,9] interaction between absorbing and scattering atoms with contributions from atomic neighbors is characterized by an AEP *V(x).*[7,9] Therefore, this effective pair potential describes not only the pair interaction of the absorber and backscatter atoms but also how their near-neighbor atoms affect such interactions. This is the difference between the AEP of this study and the single-pair potential[6] and single-bond potential,[1] which consider only each pair of immediate neighboring atoms. We assign the host atom the indicator 1 and the substitute atom the indicator 2, we have

$$V_E(x)=V(x)+\sum_{i=0,1}\sum_{j\neq i}V\left(\frac{\mu}{M_i}x\hat{\mathrm{R}}_{01}.\hat{\mathrm{R}}_{\mathrm{ij}}\right)\approx D_{12}\left(-1+\alpha_{12}^2x^2-\alpha_{12}^3x^3+\frac{7}{12}\alpha_{12}^4x^4...\right), \quad (1)$$

where i, j, μ, and $\hat{\mathrm{R}}$ is known[7,9], D_{12} is the dissociation energy, α_{12} is width of the potential. From Eq. (1), to derive analytical formula for the DWF, use perturbation theory,[9] with correlated Einstein frequency and temperature ω_E, θ_E, we obtain the DWF:

$$\sigma^{(2)}=(\hbar\omega_E/10D_{12}\alpha_{12}^2)[(1+\exp(-\theta_E/T))/(1-\exp(-\theta_E/T))], \quad (2)$$

III. RESULTS AND DISCUSSION: The calculated and experimental[4] values as in Table.

Crystal	D_{12}(eV) pres.(exp.[4])	α_{12}(Å^{-1}) pres.(exp.[4])	k_{eff}(eVA^{-2}) pres.(exp.[4])	k_{3eff}(eVA^{-3}) pres.(exp.[4])	k_{4eff}(eVA^{-4}) pres.(exp.[4])	$\omega_E(10^{13}Hz)$	$\theta_E(K)$
Cu-Cu	0.3429 (0.3528)	1.3588 (1.4072)	3.1655 (3.4931)	1.0753 (1.2289)	0.6646 (0.8070)	3.0889	236
Ag-Ag	0.3323 (0.3253)	1.3690 (1.3535)	3.1139 (2.9797)	1.0657 (1.0083)	0.6809 (0.6368)	3.3933	176
Zn-Zn	0.1698 (0.1804)	1.7054 (1.7000)	2.4692 (2.4348)	1.4889 (1.0348)	0.8378 (0.8209)	2.6868	206
CuAg72	0.3381	1.3634	3.1423	1.0710	0.6814	2.6874	207
CuZn45	0.2650	1.4672	2.8522	1.0462	0.7163	2.9161	223

Substituting the values from Tables into Eqs. (1),(2),(3), we obtain expressions for the AEP, which, and the DWF which depend on the DR and T.

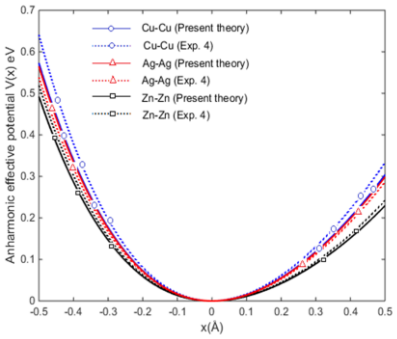

FIG. 1. AEP of Morse

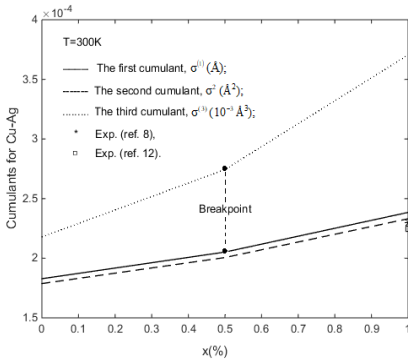

FIG. 2. Cumulants depend on DR

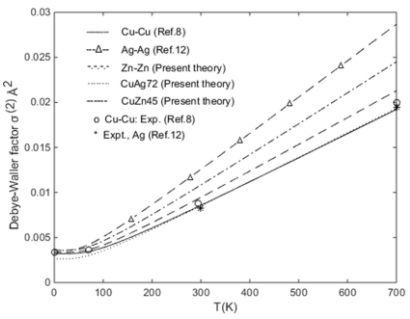

FIG. 3. DWF depend on T and DR

In Figure 1, we compare the calculated AEP Morse (solid lines) and experimental data (dotted lines) from H.Ö. Pamuk and et. al[4], for Cu (blue curve with symbol ○), Ag (red, Δ), and Zn (black, □). The calculated curves of AEP Morse align closely with the experimental curves, indicating that calculated data from the ACEM, are in good agreement with experimental values. Fig. 2 shows the first-three cumulants depend on DR at 300 K, for Cu-Ag. The graphs of $\sigma^{(1)}(T)$, $\sigma^{(2)}(T)$, and $\sigma^{(3)}(T)$ illustrate that for DRs of zero to below 50% and from over 50% to 100%, the cumulant values are proportional to the DR. For the DWF, at the point where the ratio of Ag atom decreases to 0% and the ratio of Cu atoms increases to 100% (symbols *, □), the calculated value is in good agreement with experimental. [5,12] However, there are breakpoints in the lines at the 0.5 point on the *x* axis, meaning that we do not have ordered atoms at a DR of 50%. Thus, Cu-Ag alloys do not form an ordered phase at a molar composition of 1:1, i.e., the CuAg50 alloy does not exist. This result is in agreement with the findings of J. C. Kraut and W. B. Stern.[5]

Figure 3 shows dependence of the DWF on T and DR, and comparison with the experimental values.[8,12] There good agreement at low temperatures and small differences at high temperatures for CuAg72 and CuNi45 with Cu values are reasonable. Furthermore, graphs demonstrate that the alloys of two Cu-Zn elements with Zn content less than or equal 45% enhances the durability and ductility of copper alloys, when the Zn content exceeds 50% in the Cu-Zn alloy, it becomes hard and brittle. Alloy CuZn45 is often used as heat sinks, ducts and stamping parts because of its high viscosity.[11] Also, CuAg72 is an eutectic alloy, primarily used for vacuum brazing.[10]

IV CONCLUSIONS: The expressions of the AEP, DWF received agree with all the standard properties of these quantities. Reasonable agreement with experimental and other studies has proved that this study is effective for calculating and analyzing based on the EXAFS theory.

REFERENCES

1. A. I. Frenkel and J. J. Rehr, Phys. Rev. B **48**, 585 (1993).
2. B. S. Clausen, et. al, J. Catal. **141**, 368 (1993).
3. Duc B.N., et.al, Adv. in Mat. Sci. and Eng., Vol 2018, Article ID 3263170, (2018).
4. H.Ö. Pamuk and T. Halicioğlu, Phys. Stat. Sol. **A 37**, 695 (1976).
5. J. C. Kraut and W. B. Stern, J. Gold Bulletin **33**(2), 52 (2000).
6. J. M. Tranquada and R. Ingalls, Phys. Rev. B **28**, 3520 (1997).
7. N. V. Hung, N. B. Duc, and R. R. Frahm, J. Phys. Soc. Jpn. **72**(5), 1254 (2002).
8. N. V. Hung, N. B. Duc, IWOM'S99, 1999. (12)
9. N.B. Duc, H.K.Hieu, N.T.Binh, and K.C.Nguyen, Sci. and Tec. Pub. Hou., Hanoi, 2018.
10. A.Nafi, M.Cheikh, and O.Mercier, J. of Adh. Sci. and Tec. **27** (24), 2705 (2013).
11. M. A. Laughton and D. F. Warne, Elsevier, ISBN: 978-0-7506-4637-6, 2003, pp.10.
12. N. V. Hung and N. B. Duc, Commun. in Phys., 10, (2000), pp.15-21.