Influence of Pseudo-Potential Approximation in Temperature Dependence of Residual Electrical Resistivity of Cu-Au

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Abstract

Pseudo-potential form factors developed by Animalu in 1973 were used to re-examine the problems of temperature dependence of residual electrical resistivity of Cu-Au system in the light of state of distortion and thermal vibration of the lattice along with the short-range-order of atoms above critical temperature. The Ziman"s formula for resistivity obtained yields a unified version for the calculation of resistivity in Pseudo-potential approximation. In this framework, the temperature dependence of the quantity $\Delta\rho/\rho$ for Cu-Au system was found to be in better agreement with the experimental data as compared to previous calculation.

Key Words: Influence, Pseudo-Potential, Temperature Dependence, Residual Electrical Resistivity, Cu-Au

Introduction

In general, electrical resistivity of metals increases with temperature, while the resistivity of semi conductor‘s decreases with increasing temperature. In both cases electron-phonon interaction can play a key role (Ezenwaka, 2007). The temperature dependence of the resistivity ρ of a metal is given by the Bloch- Gruneisen formula

$$\rho_{(T)} = \rho_O + A[T]_R^n \int_0^{\theta_R/T} \frac{x^n}{(e^x+1)(e^x-1)}\ \partial x \qquad (1)$$

Where ρ_O is the residual resistivity due to defect scattering and θ_R is the Debye temperature. As the temperature of the metal is sufficiently reduced, the resistivity usually reaches a constant value, known as the residual resistivity.

Success of the Pseudopotential theory of metal in calculating the structural as well as physical properties of alloys are of importance (Harrison, 1966). To analyze the contribution of long-range and short-range order to the residual electrical resistivity below and above the order -disorder critical temperature, respectively, the pseudopotential theory was used. In last few years, Sattar (2003), Yoshitake *et al*. (1987), and Oli (1986) have investigated the temperature dependence of residual electrical resistivity in Cu-Au system. Sattar (2003) has re-examined the temperature dependence of residual electrical resistivity in Cu-Au system by expanding the scattering matrix element in the Ziman formula for resistivity.

Using pseudo-potential form factors due to Animalu (1973), Sattar calculated the resistivity for three-stoichiometric compositions Cu_3Au, CuAu and $CuAu_3$ of Cu-Au system. His results showed a decrease in resistivity for Cu_3Au and CuAu alloys and increase for $CuAu_3$ as the temperature of these alloys is increased. The decrease of resistivity with the increase of temperature in Cu_3Au and Cu-Au system was found to be as expected on physical growth. At sufficiently high temperature of solid, conduction electrons in the crystal experience a rather weak statistical average crystal potential. This becomes strong with the onset of small domain with short-range-order in the alloy when the annealing temperature of the alloy is lowered with the result that the resistivity increases.

Residual Electrical Resistivity of Cu –Au System

The resistivity of the pure metal is given by Ziman's formula:

$$\rho = \frac{3\pi\Omega_o}{8he^2}\frac{m_n}{E_f}\int_0^2 \left|\langle \vec{k}+q|\vec{W}|\vec{k}\rangle\right|^2 x^2\,\partial x \quad (2)$$

Where $\langle \vec{k}+q|\vec{W}|\vec{k}\rangle$ is the matrix element of the crystal potential between two Bloch states $\langle k|$and $|\vec{k}+\vec{q}\rangle, X = \frac{q}{K_f}$, KF is the Fermi momentum and q is the scattering vector, E_f is the Fermi energy, Ω_o in the atomic volume per ion, m is the mass and ρ is

the charge of the electron, h is the Planck constant and n is the number of ions in the crystal.

For a binary alloy with short-range order and size effect of the atoms the quantity $\left|\langle \vec{k}+q|\vec{W}|\vec{k}\rangle\right|^2$ can be expanded using essentially Flinn's notation (Flinn, 1956) as

$$\left|\langle \vec{k}+q|\vec{W}|\vec{k}\rangle\right|^2 = \sum e^{iq}\left(R_m - R_m^1\right)\langle k+q|W_i|k\rangle + \sum e^{iq\frac{(R_m - R_m^1)}{N}}\{\langle\sigma_i\rangle - \sigma_i\}\, X e^{iq}\langle k+q|\Delta W|k\rangle \quad (3)$$

Where R_m is the Bravias lattice vector of atom m and m_i and the occupation operatorsσ_i are defined as follows

σ_i = M_B, if an A –atom is at R_m = M_A, if a B –atom is at R_m

Where $m_i$is the concentration of the i^{th} component. Further, we define an average potential $W_i$in equation (3) as

W_i=**M_A W_A + M_B W_B**

Which is periodic and a ―difference potential‖

= **W_A - W_B**which is disordered.

Since one knows that the microstructure responsible for the appearance of diffuse SRO (Short Range Order) scattering maxima and the Bragg peak represents the dominant conduction electron scattering in disordered alloys one can easily identify the scattering potential (the pseudo-potential form - factors) with the atomic scattering factor f. Allowing. The interatomic distances through small distortions. ∑mm1 is given by

W_{AA}^i = $r_i\left(1+\epsilon_{AA}^i\right)r_{AB}^i$ = $r_i\left(1+\epsilon_{AB}^i\right)$, and r_{BB}^i = $r_i\left(1+\epsilon_{BB}^i\right)$

Where r_i is the average distance between two lattice points and following the lines of Warren (1951), one can easily generalize the expression for residual resistivity of a binary polycrystalline solid solution.

$$\rho = \frac{3x\Omega_o}{8h e^2}\frac{m_n}{E_f} \quad N M_A M_B \int_0 \left|X\Delta W_{(q)}\right| S_{(q)}\delta x \qquad (4)$$

Where

$$S(q) \quad \Sigma_i z_i \Delta\theta\alpha_i[\sum_i z_i \alpha_i j_o(q_i r) - \sum_i z_i \beta_i j_o\{(qr) - \cos qrx\}] \qquad (5)$$

Where j_0 (qr_i) are the zero order Bassel function, Z_i and r_i the co-ordination number and radius of the i^{th} co-ordination sphere and $\propto_i$ and B_i are the lowly short-range-order and size-effect parameter, respectively. The size-effect parameter due to Warren (1951) can be expressed as

$$B_1 = \left(\frac{1}{n-1}\right)\left\{\left(\frac{M_A+\alpha_l}{M_B}\right)\epsilon^{I}_{AA} + \left(\frac{M_A+\alpha_l}{M_B}\right)\eta\,\epsilon^{I}_{BB}\right\} \text{ (6) Where}$$

$$\eta = \frac{W_B}{W_A}$$

To include the effect of thermal vibrations on the elastic structure factor S_0 (q), a Debye-Waller damping factor e^{-2m} is included so that the structure factor becomes.

$$S_{(q)} = S_0(q)e^{-2m} + A_{(q)}(e^{-2m}) \qquad (7)$$

Table 1. The Composition Dependence of the Distortion Parameters Σ_{AA} and Σ_{BB}

Cu (at %)	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Au (at%)	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1
ϵ_{AA}	-0.104	-0.093	-0.083	-0.073	-0.062	-0.049	-0.023	-0.025	-0.116
ϵ_{BB}	0.012	0.024	0.037	0.047	0.061	0.074	0.087	0.100	0.116

Method of Calculation

The integration appearing in Eq. (4) was performed using Simpson's integration scheme. The values of distortionparameters ϵ_{AA} and ϵ_{BB} are obtained by comparing the cell dimensions of the alloy with those of the A and B constituents. The values of ϵ_{AA} and ϵ_{BB} depend on concentration and are given in table 1 for Cu-Au system. The pseudopotential form factors due to Animalu (1973) were used in our calculation.

Discussion

The present calculation exhibit a decrease in the absolute values of SRO parameters as the annealing temperature of this alloy goes from 405^0C to 550^0C. We observed that the absolute value of α_1 increases as the temperature parameters of CU_3AU changes from 405^0C to 460^0C, and the temperature of the quantity $\Delta\ell/\ell$ for CU-AU system in found to be 1.4%. This value is in better agreement with the experimental one as compared to that obtained by Wang and Amar (1970).

Using the SRO parameters in the structure factor (eq.5) and the same pseudopotential form – factors due to Animalu, we find that the inclusion of the thermal vibration and static distortion of the lattice in the theory certainly improves the agreement between theory and experiment for Cu_3Au, as obtained earlier by Wang and Amar. Considering the case of CuAu one notices a decrease in the absolute values of the SRO parameters $\propto_i$ as the annealing temperature of this alloy goes from 425^0C to 525^0C. Such a decrease ought to bring a reduction in the peak height of the structure factor and this must reduce the value of resistivity in this alloy as the temperature increases.

With the inclusion of thermal lattice vibration and static lattice distortion effects in the calculation procedure of Wang and Amar, one finds a 0.5% change in the value of residual electrical resistivity as compared to 1.7% obtained earlier by Wang and Amar as the temperature rises from 425^0C to 525^0C.

Finally, one observed that in case of Cu_3Au except for the absolute value of α_I which increase as the temperature increases from 250^0C to 320^0C (Batterman, 1996) in contrast to the other experimental results for Cu_3Au and CuAu, the absolute value of $\alpha_I>1$ decreases with the increase in temperature, and using the same reasoning one expects a decrease in the value of residual electrical resistivity of this system as the temperature goes from 250^0C to 320^0C. In fact, a sharp decrease has been measured in this alloy as temperature rises from 190^0C to 350^0C. Contrary to Wang and Amar who obtained a rise in the value of $\rho(T)$ as temperature increase from 250^0C to 320^0C. Our calculation with the same pseudo potential form factor due to Animalu and Batterman‘s experimental data with the inclusion of thermal vibration and static distortions of the lattice, however, yielded a decrease of 2.8% in the value of $\Delta\rho/\rho$ as the temperature

varied from 250^0C to 320^0C, which is in agreement with the experimental results for this system.

Conclusions

In conclusion, extended pseudo potential approximately provides a unified framework for the description of residual electrical resistivity in disordered solid solutions. Moreover, the procedure described gives a better agreement with the experimental data for the temperature dependence of $\rho(T)$ when applied to the case of Cu-Au systems.

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