THE CONTRIBUTIONS FROM SHORT-RANGE ORDER AND THE SIZE EFFECT TO Cu-Zn ALLOY RESISTIVITY

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A model potential has been used in calculating the residual resistivity for Cu + 15 at.% Zn. The size effect has an anomalous influence on the residual resistivity in Cu-Zn alloys (reduces it).

It is usually assumed that the resistivity ρ of a metal or solid solution is governed by a combination of the valency and size effects, where it increases with the differences in the component valencies and atomic sizes [1]. Long-range order should reduce the resistivity by 20-30%, as should short-range order in the absence of anomalies, but to a smaller extent (up to 10%). The usual pseudopotentials [2] used in calculations on ρ do not give reasonable agreement with experiment, particularly for transition metals, so a theoretical analysis of factor effects is used mainly to elucidate the nature of the anomalies such as the increase in ρ on annealing a deformed solid solution [3]. New pseudopotentials [4,5] have given interest to the theory of solution resistivity in relation to the size effect and short-range order. Here we show that certain common assumptions are incorrect from a theoretical analysis of how these factors influence Cu-Zn alloys.

The pseudopotential method was used with the measured [6] short-range order and size-effect parameters. The pseudopotential form factor for a nontrasition metal was taken from [2], while we used [4] for a noble metal, with the pseudopotential screening employed in the [5] model, and the nonresonant parts calculated in the quasilocal approximation, and the resonant ones from the complete nonlocal theory. We calculated ρ from

$$\rho=\frac{3\pi\Omega_0 m}{8\hbar e^2 E_F}\, c_A c_B \int_0^2 \sum_i \alpha(\rho_i) e^{iq\rho_i} |\Delta W(q)-(qA_Q)\overline{W}(q)|^2 x^3 dx. \qquad (1)$$

The results are as follows. In a disordered solid solution, the resistivity due to the valency difference is

$$\rho_v^0=\frac{3\pi\Omega_0 m}{8\hbar e^2 E_F}\, c_A c_B \int_0^2 |\Delta W(q)|^2 x^3 dx \qquad (2)$$

and is 2.8 μΩ·cm, while that due to the size effect,

$$\rho_{se}=\frac{3\pi\Omega_0 m}{8\hbar e^3 E_F}\, c_A c_B \int_0^2 [-2\Delta W(q)\overline{W}(q)\langle qA_Q\rangle_{\theta,\varphi}+|\overline{W}(q)|^2 \langle qA_Q\rangle_{\theta,\varphi}^2]\, x^3 dx \qquad (3)$$

is -0.6 μΩ·cm, and that due to the short-range order is also -0.6 μΩ·cm. This ρ is close to the observed 2.6 μΩ·cm, so one can examine how the size factors contribute to ρ.

The size effect and the short-range order in Cu-Zn reduce ρ by more than 20%, which is fairly unexpected. The change in ρ due to the short-range order is substantially larger than the usual values, but even more interest attaches to the considerable reduction in ρ from the combination of the two effects, which has not been discussed previously. The magnitude of this may be even larger for other solid solutions because it is dependent on the factor $\frac{1}{v}\frac{\partial v}{\partial c}$ appearing in the expression for A_Q $\left(A_Q \sim \frac{(1+\sigma)}{3(1-\sigma)}\frac{1}{v}\frac{\partial v}{\partial c}\frac{Q}{Q^2}\right)$, where Hume-Rothery's rule gives $\frac{1}{v}\frac{\partial v}{\partial c} = 0{,}4$ even for unrestricted solid solutions, whereas $\frac{1}{v}\frac{\partial v}{\partial c} = 0{,}18$) for Cu-Zn.

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