ELECTRICAL RESISTIVITY OF A DISORDERED Pd—Si ALLOY[1]

ЭЛЕКТРИЧЕСКОЕ УДЕЛЬНОЕ СОПРОТИВЛЕНИЕ НЕУПОРЯДОЧЕННОГО СПЛАВА Pd—Si

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The electrical resistivity of a disordered Pd—Si alloy has been calculated by means of the t-matrix formulation of the Ziman theory. The relationship of the theoretical results to the experimental work on the $Pd_{80}Si_{20}$ alloy is discussed.

We shal use the approximation of nearly free electrons with scattering described by the t-matrix of a model muffin-tin potential for the calculation of the electrical resistivity of an amorphous Pd—Si alloy. Similarly as in [1] we suppose that only the s-electrons of the transition metal, together with the valence electrons of the metalloid atoms, take part in the electrical conductivity. The electrical resistivity in such a case can be expressed as

$$\varrho = \frac{2\pi\Omega_0}{e^2\hbar v_F^2}\int_0^1 \mathrm{d}\left(\frac{q}{2k_F}\right)\frac{q}{2k_F}\,|\langle \boldsymbol{k}_F'|T|\boldsymbol{k}_F\rangle|^2. \tag{1}$$

The T-matrix for a two-component alloy is given by

$$|\langle \boldsymbol{k}_F'|T|\boldsymbol{k}_F\rangle|^2 = c_1|t_1(E_F, q)|^2[1-c_1+c_1a_{11}(q)] + c_2|t_2(E_F, q)|^2\times$$
$$\times[1-c_2+c_2a_{22}(q)] + c_1c_2(t_1t_2^* + t_1^*t_2)[a_{12}(q)-1], \tag{2}$$

where c_1, c_2 are concentrations of the components, Ω_0 is the atomic volume and v_F, E_F are the Fermi velocity and the Fermi energy, respectively. k_F, the free electron wave number, is given by $k_F^3 = 3\pi^2 Z/\Omega_0$, where $Z = Z_1c_1 + Z_2c_2$. Z, Z_1, Z_2 are the effective valences of the alloy and the components. The T-matrix (2) is expressed in terms of the partial structure factors $a_{11}(q)$, $a_{12}(q)$, $a_{22}(q)$ as well as of the single-site t-matrices. The structure factors depend on the geometrical distribution of the scattering centres, while $t_i(E_F, q)$, $(i = 1, 2)$ describes the scattering of an electron from a state $\boldsymbol{k}_F$ to a state $\boldsymbol{k}_F' = \boldsymbol{k}_F + \boldsymbol{q}$ by the following relation

$$t_i(E_F, q) = -\frac{2\pi\hbar^3}{\Omega_0 m_0\sqrt{2m^*E_F}}\sum_{l=0}^{\infty}(2l+1)\sin\delta_l^i(E_F)\exp[i\delta_l^i(E_F)]\times P_l(\cos\Theta), \tag{3}$$

where $q = |\boldsymbol{k}_F' - \boldsymbol{k}_F|$, $\delta_l^i(E_F)$ are the phase shifts at the Fermi energy and P_l are the Legendre

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polynomials. The phase shifts $\delta_l^i(E_F)$ can be determined by solving the radial Schrödinger equation with the model muffin-tin potential. We have calculated with the potential defined by B. Vasvari as [2]

$$V_{MMTP}(r) = \begin{cases} \dfrac{-2Z_i \exp[Ar(r-2r_m)]}{r} - V_{AVE} & \text{for } r<r_m \\ 0 & \text{for } r>r_m \end{cases} \tag{4}$$

where Z_i is the charge of the nucleus, A is the adjustable parameter, r_m the muffin-tin radius and V_{AVE} the muffin-tin constant. For the determination of the structure factors $a_{11}(q)$, $a_{22}(q)$ we have used the Percus-Yevick approximation [3]. The factor $a_{12}(q)$ is taken from diffraction experiments [4]. As it is difficult to determine the effective valences of the components, we have calculated two variants: e) Effective valence $Z_{Pd}=0$, $Z_{Si}=4$. b) $Z_{Pd}=0.36$, $Z_{Si}=4$.

Table 1

Parameters of the model muffin-tin potential and results for amorphous metallic Pd—Si glasses. The parameters of the potential for Pd and Si (in at. units) $A_{Pd}=0.612$ a.u., $r_{mPd}=2.598$ a.u. $A_{Si}=0.576$ a.u., $r_{mSi}=2.304$ a.u.

c_{Si}	$Z^{(a)}$	$\varrho^{(a)}_{teor}$ [μΩm]	$Z^{(b)}$	$\varrho^{(b)}_{teor}$ [μΩm]	ϱ_{exp} [μΩm]
0.15	0.60	0.25	0.906	0.37	—
0.17	0.68	0.30	0.978	0.49	0.71
0.20	0.80	0.47	1.098	1.10	1.09
0.23	0.92	0.88	1.197	1.28	—
0.25	1.00	1.00	1.27	1.48	—

The parameters used in the calculation, as well as the obtained theoretical results together with the experimental data [5] are summarized in Table 1. We can see that in the case of the second variant the experimental values are in good agreement with the theoretical results. It means that the second variant is a more realistic model for the Pd—Si alloy.

REFERENCES

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