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Electrical resistivity of liquid Mg–Al, Na–Cs, Ni–Ce, Li–Cd and Mg–Cd alloys within the ‘ $2k_F$ ’ scattering model

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Abstract

The resistivities of liquid Mg–Al, Na–Cs, Ni–Ce, Li–Cd and Mg–Cd alloys were calculated. The Faber–Ziman diffraction model and the Morgan–Howson–Šaub ‘ $2k_F$ ’ scattering model were used in calculations. The results obtained within these two models for the same alloy and with use of the same set of parameters differ substantially, even for alloys that are not highly resistive. It is possible in principle to achieve good agreement with experiment by means of each of these two models; however we suggest that the ‘ $2k_F$ ’ scattering model is the appropriate method of calculation of the electrical resistivity for liquid alloys because the quantum interference effects should always be taken into account.

1. Introduction

Electrical resistivity of liquid alloys has been a subject of interest for many years. In theoretical approaches mostly the Faber–Ziman (FZ) [1, 2] model has been used [3–5]; however it includes quantum effects only in the first Born approximation. In particular, it neglects multiple scattering that leads to quantum interference. As was shown in [6], the quantum interference has a strong effect on the resistivity of binary alloys; therefore it must not be neglected in theoretical calculations. Actually, for every disordered system with resistivity greater than about $50 \mu\Omega \text{ cm}$ the FZ model is no longer valid and better quantum models should be used (in some cases quantum interference gives a rather small contribution to the resistivity even up to about $100 \mu\Omega \text{ cm}$ but it is more appropriate to use a quantum model).

In 1985 the ‘ $2k_F$ ’ scattering model was proposed by Morgan, Howson and Šaub [7] (it is also called the MHS model). It was based on the quantum kinetic equation and gave formulae for the resistivity that included the quantum interference effect. This model allowed performing calculations for highly resistive alloys, such as amorphous Ca–Al or liquid K–Cl, in which the localization (in the Bergman sense [8]) occurs [6, 9].

In this paper we present successful calculations of the resistivity with use of the MHS model for several liquid alloys

that were previously analyzed by means of the FZ model (except for Mg–Al and Na–Cs for which some calculations with the MHS model were performed [10]). We also include the Debye–Waller factor to take into account the temperature dependence of the partial structure factors, which has usually been neglected, except in the work [11].

2. ‘ $2k_F$ ’ scattering model

The resistivity in the ‘ $2k_F$ ’ scattering model is given by the formula [9]

$$\rho = \frac{m_e^*}{ne^2\tau_{tr}}, \quad (1)$$

where the transport lifetime τ_{tr} is expressed as [7]

$$\frac{1}{\tau_{tr}} = \frac{1}{\tau_{FZ}} \frac{1 + \frac{1}{2} \frac{\tau_{FZ}}{\tau} X^2 F_{MHS}^{1/2}(X)}{1 - \frac{3}{64} X^4 F_{MHS}(X)}. \quad (2)$$

Here τ_{FZ} is the transport lifetime and τ is the one-electron lifetime (both taken from the FZ model), $X = \hbar/(\tau E_F)$ and

$$F_{MHS}(X) = \left[2 \ln \frac{(1 + X^2)^{1/2} + 1 + 2^{1/2} [(1 + X^2)^{1/2} + 1]^{1/2}}{(1 + X^2)^{1/2} + 1 - 2^{1/2} [(1 + X^2)^{1/2} + 1]^{1/2}} \right]^2. \quad (3)$$

The FZ model lifetimes for binary alloy are expressed as [6]

$$\frac{1}{\tau_{\text{FZ}}} = \frac{m_e^* \Omega_0}{4\pi \hbar^3 k_F^3} \int_0^{2k_F} dq \lambda(q) q^3 \quad (4)$$

$$\frac{1}{\tau} = \frac{m_e^* \Omega_0}{2\pi \hbar^3 k_F} \int_0^{2k_F} dq \lambda(q) q \quad (5)$$

where Ω_0 is the average volume per one atom in the system, and

$$\lambda(q) = \sum_{\alpha=1}^2 \sum_{\beta=1}^2 \sqrt{c_\alpha c_\beta} S_{\alpha\beta}(q) u_\alpha(q) u_\beta(q). \quad (6)$$

In this equation c_i stands for the number concentration of the i th component, $u_i(q)$ are the screened pseudopotentials' form factors and S_{ij} are the Ashcroft–Langreth partial structure factors [12].

3. Details of calculations

For calculation of the partial structure factors the algorithm from the Waseda book [13] was used, corrected with the Debye–Waller factor. Denoting the original Ashcroft–Langreth factors given by the Waseda algorithm as S_{ij}^0 we introduce the Debye–Waller factor following reference [11]:

$$S_{ij}(q) = \delta_{ij} + (S_{ij}^0(q) - \delta_{ij}) \exp[-2W(q)] \quad (7)$$

where

$$W(q) = \frac{3\hbar^2 q^2 T^2}{2Mk_B \theta_D^3} \int_0^{\theta_D/T} dx \left(\frac{1}{\exp(x) - 1} + \frac{1}{2} \right) x, \quad (8)$$

M is the average ion mass of the system and θ_D is the Debye temperature.

Fitting the calculated structure factors for single-element liquids to experimental data [13] we determined the hard sphere diameters for use in further calculations.

In the resistivity calculations two model pseudopotentials were used: the Heine–Abarenkov (HA) one for each element and the Shaw one for Mg and Al only (tabulated in [14]). Such a choice was made to present both a comparison of using two different pseudopotentials, and the possibility of using the MHS model for calculation of the resistivity for various alloys. At the present time there are available *ab initio* pseudopotentials but they are as strongly parametrized as simpler model pseudopotentials; therefore we decided to use the second ones.

The unscreened form factor for HA pseudopotential is expressed as [15]

$$u^b(q) = -\frac{1}{\Omega_0 \epsilon_0} \frac{q(Ze^2 - AR_c) \cos(qR_c) + A \sin(qR_c)}{q^3}. \quad (9)$$

Here R_c is a cutoff radius and A is the well depth, and these are the only two parameters of this pseudopotential. Their values were used as fitting parameters.

The screened pseudopotential form factor is expressed as $u(q) = u^b(q)/\epsilon(q)$, where $\epsilon(q)$ is a dielectric function taken in the Hartree form [16]:

$$\epsilon(q) = 1 + (\epsilon_H(q) - 1) \times (1 - G(q)) \quad (10)$$

Table 1. Parameters used in calculations. The hard sphere diameters σ were estimated from fitting to the experimental structure factors (figure 1). R_c and A are the parameters of the pseudopotentials (a lack of a value means that the pseudopotential was taken from [14]). Debye temperatures θ_D were taken from [24]; for Ce the value was interpolated.

Alloy, T (K)	Element	σ (au)	R_c (au)	A (au)	θ_D (K)
(a) Al–Mg	Al	4.87	—	—	428
770	Mg	6.50	—	—	400
(b) Al–Mg	Al	4.87	3.3	1.5	428
770	Mg	6.50	1.5	0.35	400
(c) Li–Cd	Li	5.32	4.5	0.095	344
820	Cd	5.22	3.0	0.6	209
(d) Mg–Cd	Mg	5.46	1.5	0.35	300
970	Cd	5.22	3.0	0.6	209
(e) Na–Cs	Na	6.50	3.8	0.26	158
400	Cs	9.35	7.5	0.14	38
(f) Ni–Ce	Ni	4.24	2.66	0.26	450
1770	Ce	5.82	2.4	0.43	120

where $\epsilon_H(q)$ is the Hartree static dielectric function:

$$\epsilon_H(q) = 1 + \frac{m_e^* e^2}{2\pi k_F \hbar^2 Q^2} \left(\frac{1 - Q^2}{2Q} \ln \left| \frac{1 + Q}{1 - Q} \right| + 1 \right) \quad (11)$$

and $Q = q/(2k_F)$. $G(q)$ is a correlation function for which several forms were proposed [16]. For resistivity calculations the Ishimaru–Utsumi [17] form was chosen.

The value of the mean density and the Debye temperature for the alloys investigated were taken as linear functions of the concentration. Although these are not precise dependences we do not expect any substantial influence of this approximation on the final results because the dependence of the results on pseudopotentials is much stronger.

The density of the conduction electrons, the Fermi energy and vector, and the volume per atom were taken from the free electron model [18], and the packing fraction of the system was calculated in the same way as in [11]:

$$\eta = \frac{1}{6} \frac{1}{\Omega_0} \pi [\sigma_1^3 (1 - c) + \sigma_2^3 c] \quad (12)$$

where σ_1, σ_2 stand for hard sphere diameters.

Effective electron masses were assumed to be equal to unity (in atomic units), which should be true for most metals. We do not expect significant deviations from this value and even then the influence should be much smaller than that arising from the choice of pseudopotential parameters.

We performed the fitting of the MHS formula for the resistivity (equations (1) and (2)) to the experimental data.

The only parameters used for fitting the curves were the parameters of the pseudopotentials. Other values were taken from tables or calculated. All values used in our calculations are summarized in table 1.

4. Results

Hard sphere diameters were obtained from fitting experimental and calculated structure factors for pure liquid elements. Both experimental data and results of our calculations are presented

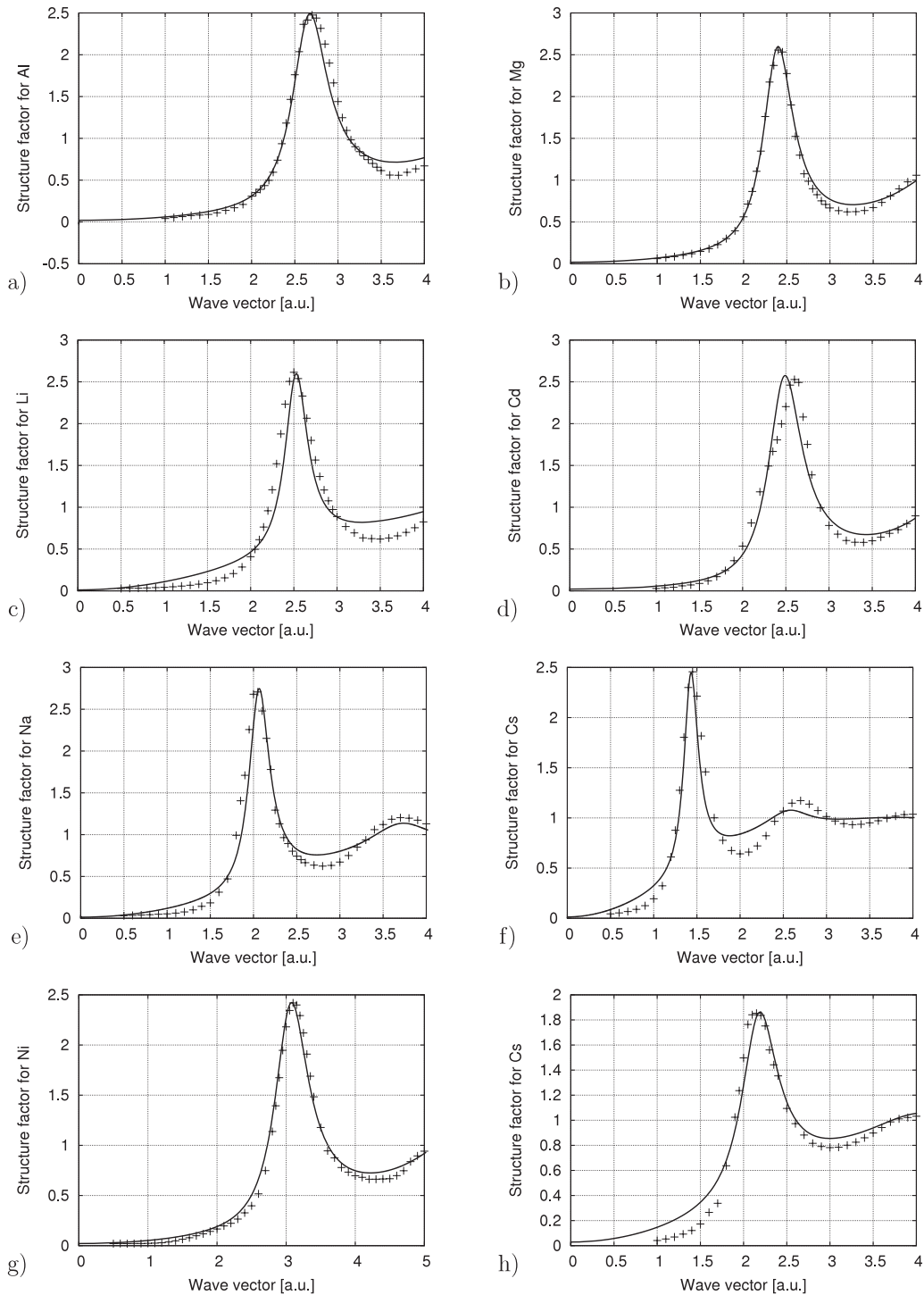


Figure 1. Structure factors calculated for each element (line), with experimental values taken from [13] (crosses): (a) Al, (b) Mg, (c) Li, (d) Cd, (e) Na, (f) Cs, (g) Ni, (h) Ce.

in figure 1, whereas the values of the hard sphere diameters obtained are shown in table 1. The fittings were performed to the data obtained in the temperatures as near as possible to the ones applied in further calculations. The assumption that diameters do not change with temperature was made. Although this is only approximately true, it should not have a significant effect on the resistivity calculations and affect the main point of this work.

The results of our calculations are shown in figure 2, together with experimental data taken from the literature. In figures 2(a) and (b) (both for Al–Mg) we can see the difference coming from using two different pseudopotentials: the Shaw pseudopotential (2(a)) and the HA one (2(b)). We can see that the latter gives a slightly better approximation. The lines in figure 2 representing the results for the FZ model were calculated with use of the same parameters as for plotting the

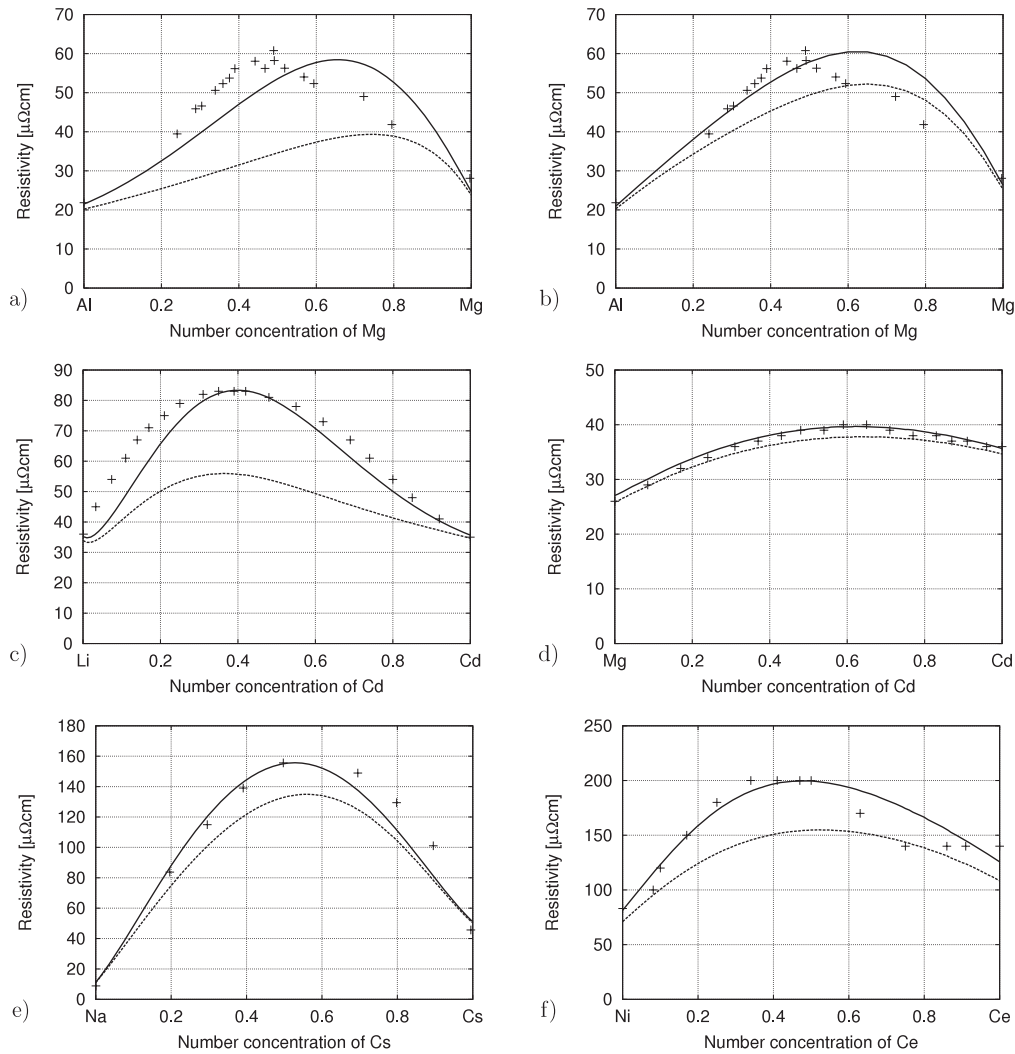


Figure 2. Calculated values of the resistivity for several liquid alloys as a function of their composition: according to the MHŠ model (solid line), and to the FZ model (dotted line). Crosses denote experimental values taken from the literature: (a) Al–Mg [19] (calculations with use of the Shaw pseudopotential), (b) Al–Mg [19] (calculations with use of the HA pseudopotential), (c) Li–Cd [20], (d) Mg–Cd [21], (e) Na–Cs [22], (f) Ni–Ce [23]. Details are given in the text.

MHŠ results. The difference between MHŠ and FZ curves shows that the contribution of the quantum interference may be significant even for the resistivity of about $50 \mu\Omega \text{ cm}$. For Li–Cd (figure 2(c)), Mg–Cd (figure 2(d)), Na–Cs (figure 2(e)) and Ni–Ce (figure 2(f)) a good agreement between the fitting lines and the experimental values was achieved by means of the MHŠ model. The FZ curves calculated with use of the same parameters apparently differ from the MHŠ ones. The largest relative difference between them is obtained for Li–Cd, the resistivity of which is smaller than $90 \mu\Omega \text{ cm}$. For Na–Cs alloy the difference between MHŠ and FZ model curves is much smaller and this suggests a rather small contribution of quantum interference despite its high resistivity (over $100 \mu\Omega \text{ cm}$).

5. Summary

There are two theoretical models which describe the electron transport in disordered media such as liquid and amorphous

alloys: the FZ diffraction model and the MHŠ model, also known as the ‘ $2k_F$ ’ scattering one. Most authors explain their experimental results by means of the FZ model. This is possible because this model is very sensitive to the choice of pseudopotential. However, this procedure is inappropriate in our opinion. The FZ model is a one-scattering theory whereas the conduction electron certainly is multiply scattered because of a very short mean free path. The effects of ‘back-scattering’ and quantum interference cannot be neglected. The MHŠ theory starts from the exact quantum transport equation and treats the above-mentioned effects in an appropriate way. We showed in our calculations that the MHŠ model agrees very well with available experimental data. The use of this model is very simple when we already have the results calculated from the FZ model. Only one step of calculations is now required to obtain more reliable results, as we have shown in our work. Therefore it is reasonable to always use a physically sound model, i.e. the MHŠ one, which takes into account multiple scattering and quantum interference, to explain electron transport properties of disordered systems.

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