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The calculation of electronic transport coefficients of metals in the process of transition from liquid to plasma

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Abstract

A recently developed method for calculation of electronic transport coefficients of liquid metals was applied to a region of transition from the liquid to the plasma state for non-alkali metals. This technique is based on Ziman theory and a two-component model of the medium with variable ion charge. The results of calculation were compared with calculations and measurements of other authors.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The calculation of wide-range transport coefficients of metals is an important task both for theory and for practical applications. So there are different calculation models for disordered states of the metals (see [1–5]). But to use these models one needs to know some parameters, the most important of which is the chemical composition of the substance under study.

The problem of chemical composition is partially solved for the gaseous (plasma) state of metals (i.e. for non-alkali metals when approximately $\rho \leq 1 \text{ g cm}^{-3}$, $T \geq 10^4 \text{ K}$) [1, 2, 5]. The liquid state of simple metals such as aluminium can be considered as a two-component mixture of positive ions and degenerate electrons in the region near melting point. Then the charge of an ion is equal to the valence of the corresponding atom [3, 4].

Neither of these approaches are valid in the transition region between liquid and plasma. The parameters of this intermediate area were obtained in recent experiments [6–8], which also stimulated the development of theory. Earlier a model of a two-component medium with variable ion charge [9] was presented, which has been applied to the description of aluminium

[10]. In this work we develop calculations with this model for aluminium and expand it for the case of copper and tungsten.

The paper is organized as follows: in section 2 the main relations of our model will be presented. In section 3 will be given results of our calculation and their comparison with theoretical and experimental data of other researchers.

2. The main relations of the model

One of the widely used approaches for calculation of liquid metal conductivity was proposed by Ziman [3]. His theory was created on the basis of solution of the scattering task for free electrons in the Born approximation. According to this theory,

$$\frac{1}{\sigma} = \frac{m_e^2}{12\pi^3 \hbar^3 e^2 n_e^2} \int_0^\infty k^3 f_0(k/2) \sum_{a,b} \sqrt{n_a n_b} \tilde{U}_{ea}(k) \tilde{U}_{eb}^*(k) S_{ab}(k) dk. \quad (1)$$

Expression (1) is written for the case of non-zero temperatures T . It also allows for the presence of several types of heavy particles (positive ions and atoms) with concentrations n_a, n_b . Here n_e is the concentration of free electrons, μ is their chemical potential, $f_0(k)$ is the Fermi–Dirac distribution function, \tilde{U}_{ea} —Fourier transform of interaction potential, S_{ab} —structure factors of heavy components.

In our model we suppose that the metal consists of only one sort of ions of charge Z , and electrons. Then ion and electron concentrations can be obtained by equality of total electron and ion charges $n_e = Zn_i$. So it is necessary to know the electron–ion potential and structure factor for conductivity calculation. In the theory of liquid metals so-called electron–ion pseudo-potentials $w_{ei}(r)$ are usually introduced. Then $\tilde{U}_e(q) = \tilde{w}_{ei}(q)/\varepsilon(q)$, where $\varepsilon(q)$ is the dielectric function of the electron subsystem [3, 4]. One of these pseudo-potentials was chosen as

$$w_{ei}(r) = \begin{cases} -A, & r < r_0 \\ -A(r_0/r), & r \geq r_0. \end{cases} \quad (2)$$

Considering that an ion consists of a nucleus of charge Z_1 (Z_1 is an ordinal number in the periodic table of elements) and a cloud of bound electrons with density $\rho(r)$ one can easily find this density, using the relation

$$4\pi\epsilon_0 w_{ei}(r) = -\frac{Z_1|e|^2}{r} + |e|^2 \int \frac{\rho(\mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|} d\mathbf{r}_1, \quad (3)$$

ϵ_0 is SI constant. Then the effective charge of ion Z^* is defined as

$$Z^* = Z_1 - \int \rho(r) dr = \frac{9\pi\epsilon_0 A r_0}{|e|^2}. \quad (4)$$

The effective ion–ion potential, in view of (2)–(4), may be calculated by the formula:

$$\Phi_{ii}(r) = \frac{(Z^*|e|)^2}{2\pi^2\epsilon_0 r} \int_0^\infty \frac{\sin^2 x \sin xr}{x^3 \varepsilon(x/r_0)} dx. \quad (5)$$

Various expressions for dielectric function ε are described in [11, 12]. (The result of [12] appeared to be optimal in our case.) Further, if the ion–ion interaction potential is known, one can find a pair correlation function (and an ion–ion structure factor) by a solution of a system of integral equations that was developed in theory of liquids [2]. In our calculations we used two closing relations: the Percus–Yevick equation and the MHNC equation. For a given interaction potential and pair correlation function one can find the interaction part of free energy by means of a well-known relation [9]. Then all quantities (2)–(5) depend on the two parameters A, r_0 . The calculation method of these parameters is also described in [9].

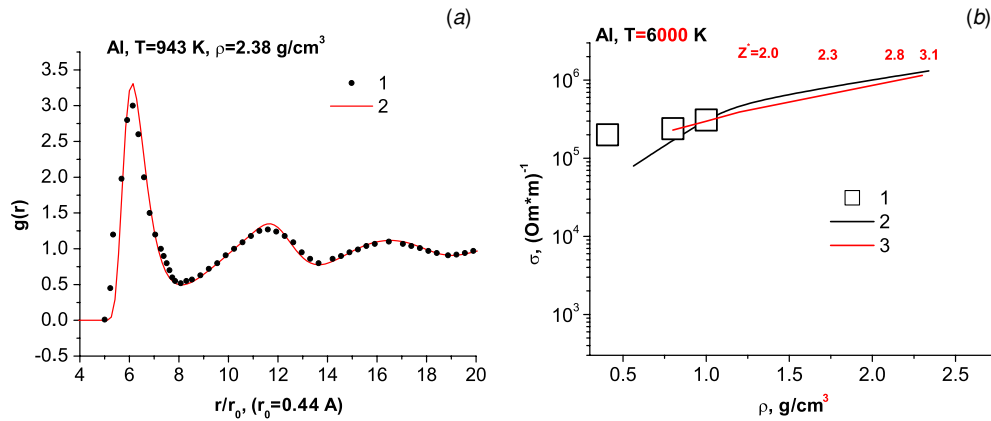


Figure 1. (a) Structure factor of liquid aluminium: 1—[13], 2—this work. (b) Conductivity of aluminium at $T = 6000$ K: 1—[6], 2—[14], 3—this work.

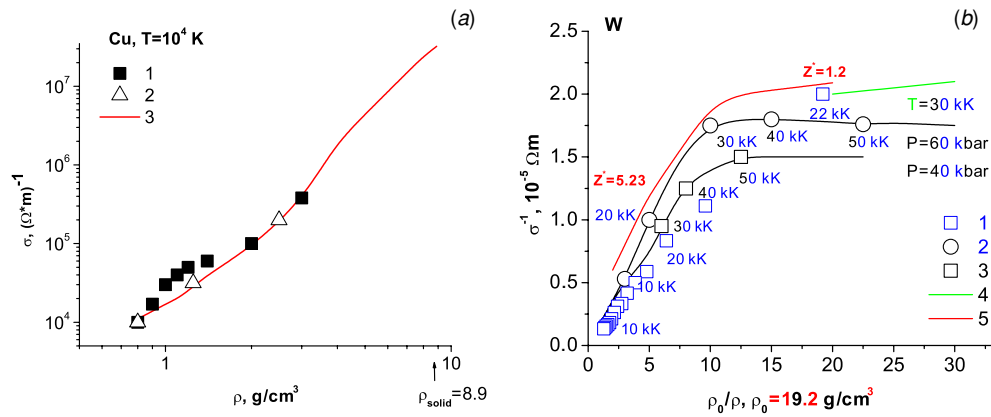


Figure 2. (a) Conductivity of copper at $T = 10000$ K: 1—[6], 2—[15], 3—this work. (b) Resistivity of tungsten according to different measurements and calculations: 1—[7], 2 and 3—[8], 4—[1], 5—this work.

3. Results

The results of calculations are presented in figures 1(a), (b) and 2(a), (b). In figure 1(a) there is a structure factor of liquid aluminium, according to our calculation and experiments [13]. In figure 1(b) there are results of calculations and measurements of conductivity of aluminium at isotherm $T = 6000$ K for a wide range of densities. The measurement error corresponds to the size of the squares. The effective charge (z^*) is also plotted in figure 1(b). There is good agreement between our data and measurements [6] as well as *ab initio* simulation [14] for $\rho \geq 1$ g cm $^{-3}$. In this region our structure factor almost coincides with measurements [13]. For smaller densities there is divergence between the experiment and calculation as well as between calculations. This fact points to the possible inaccuracy of the Born approximation, used in our model, for the case of the liquid state of metals [4]. The results of calculation and measurements of copper and tungsten conductivity are presented in figures 2(a) and 2(b),

respectively. Although copper is not a simple metal, our model gave rise to results consistent with those of the *ab initio* simulation [15] and with data of experiments [6]. For the higher temperatures (15–20 kK) our results are also in agreement with measurements [6] for Al and Cu.

For tungsten our calculation qualitatively reproduces the increase of resistivity in the process of expansion of tungsten, observed in measurements [7, 8]. In the experiment [7] resistivity, density and temperature were measured. The errors of these measurements correspond to the size of the squares. The lines with symbols are the results of wire explosion measurements (resistivity) and calculations of the MHD task for this process (density, temperature) [8]. The errors of these measurements are about 10%. The variations of temperature measured in [7, 8] are also presented in figure 2(b). The process of expansion of tungsten became isobaric in experiments [8] (the corresponding pressure is placed near each set of measurements). The authors of [8] supposed that their measurements pointed to a metal–non-metal transition. One of the explanations of this phenomenon is ionization by pressure. To check this possibility we calculated the resistivity of W for isotherm $T = 30\,000$ K. This isotherm for plasma densities is also presented in [8], according to the theory [1]. Effective ion charge (4) is also plotted in figure 2(b). Its decreasing in the process of expansion confirms the hypothesis about possible pressure ionization. We have not succeeded in quantitatively reproducing the results of [8] which indicates the possible limitation of the use of the model in hand for transition metals.

Acknowledgments

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