Materials Science-Poland, Vol. 24, No. 3, 2006

Electrical resistivity of disordered monolayer metallic films

P. JARGUZ[*], A. PAJA

Faculty of Physics and Applied Computer Science, AGH University of Science and Technology,
al. Mickiewicza 30, 30-059 Cracow, Poland

Electron transport through a disordered two-dimensional array of potentials has been investigated. The resistivity was calculated according to the Faber–Ziman diffraction model, suitably modified for a two-dimensional electron gas. The structure factor is obtained by means of numerical simulations. The pseudopotentials are assumed to be Shaw potentials with appropriate screening. The resistivities of disordered monolayers of alkali metals have been calculated in this model using parameters that allowed us to explain the experimental data for bulk materials.

Key words: *electrical resistivity; disordered system; two-dimensional electron gas*

1. Introduction

Rapid development of nanoelectronics that has been recently observed generates the need for a theoretical description of electron transport properties of nanoscale systems. Such systems have at least one size small enough that the electron wave function essentially differs from that in a bulk material. This, in turn, influences physical properties of the system.

In this work, we consider a disordered monolayer metallic film. Such films can now be obtained by the MBE technique [1, 2]. We assume that their transport properties, electrical resistivity in particular, can be described by the behaviour of a two -dimensional electron gas placed in a superposition of a static electric field and a disordered array of ionic potentials. The scattering of conduction electrons is described within the diffraction model [3]. The calculated resistivities of monolayers of alkali metals will be compared with available experimental data for corresponding bulk materials.

---

[*] Corresponding author, e-mail: jarguz@uci.agh.edu.pl

2. Theoretical model

The electrical resistivity ρ of a disordered array of ions can be calculated in a Boltzmann-type approximation using the formula

$$\rho = \frac{m}{ne^2\tau_{tr}} \tag{1}$$

where m and e are the electron mass and charge, respectively, n is electron concentration, and τ_{tr} is the transport relaxation time. In a two-dimensional picture, n is of course the area density, i.e. the density of carriers per unit area. Ziman's formula for τ_{tr} [3] should also be appropriately modified [4]:

$$\tau_{tr}^{-1} = 2\frac{v_F}{A}\int_0^{\pi} d\varphi \frac{d\sigma}{d\varphi}(1-\cos\varphi) \tag{2}$$

where v_F is the Fermi velocity and A is the area of the system. Here, $d\sigma/d\varphi$ is the differential cross section for two dimensions [4]:

$$\frac{d\sigma}{d\varphi} = \frac{1}{8\pi k_F}\left(\frac{m}{2\pi\hbar^2}\right)^2 NS(q)\left|u_a(q)\right|^2 \tag{3}$$

where k_F is the Fermi wave vector in the xy plane, N is the total number of atoms in the system, $S(q)$ is a two-dimensional structure factor, $u_a(q)$ is a two-dimensional Fourier transform of the atomic potential $u_a(\mathbf{r})$, and

$$q = 2k_F \sin\frac{\varphi}{2} \tag{4}$$

The structure factor $S(q)$ defined as

$$S(q) = \frac{1}{N}\left\langle \sum_j \sum_k \exp\left[-i\mathbf{q}\cdot\left(\mathbf{r}_j - \mathbf{r}_k\right)\right]\right\rangle - N\delta_{\mathbf{q},\mathbf{0}} \tag{5}$$

has been calculated by means of numerical simulations. We placed circles of a given diameter σ in a rectangle of a given size at random, so that they filled up the whole area but did not overlap each other, after which we computed the sum in Eq. (5). This is equivalent to using the random closely packed hard sphere model. The rectangles used in our calculations contained at least a thousand of these artificial atoms. We took the average over an ensemble of at least a thousand random configurations.

To calculate the differential cross-section, we also need an analytical form of the scattering potential. We assumed the Shaw pseudopotential, modified by screening [6]:

$$u_a(r) = \begin{cases} -\dfrac{Z}{r}\exp(-\lambda r), & r \ge R_c \\ -\dfrac{Z}{R_c}\exp(-\lambda R_c), & r \le R_c \end{cases} \tag{6}$$

where R_c is the core radius, λ is the screening parameter, and $Z=e^2/(4\pi\varepsilon_0)$ in SI units. Such a form gave good agreement with the experimental results for bulk alkali metals in our previous work [6].

Unfortunately, the Fourier transform of this potential in two dimensions

$$u_a(\mathbf{q}) = \iint u_a(\mathbf{r})\exp(-i\mathbf{q}\cdot\mathbf{r})d^2\mathbf{r} \tag{7}$$

cannot be expressed by elementary functions. We converted it into a real integral

$$u_a(q) = 4\int_0^\infty dr\, u_a(r) \int_0^{\frac{\pi}{2}} d\varphi \cos(qr\cos\varphi) \tag{8}$$

and calculated it numerically.

3. Results of calculations

We calculated the structure factors $S(q)$ given by Eq. (5) for five alkali metals: Li, Na, K, Rb, and Cs using atomic diameters taken from [7], which reproduced well the experimental structure factors for bulk samples. These values are given in Table 1. The structure factors for all five elements are shown in Fig. 1.

Table 1. Input parameters for numerical calculations and the resulting resistivities

Element	σ [10^{-10} m]	λ [10^{10} m]	R_c [10^{-10} m]	ρ_m [Ω]	ρ_b [μΩ·cm]	$\rho_{\exp}$ [μΩ·cm]
Li	2.70	1.36	0.66	55.4	1.68	25
Na	3.28	1.23	1.25	19.7	0.73	9.6
K	4.07	1.11	1.53	22.2	1.01	13
Ru	4.30	1.08	1.47	31.8	1.57	22
Cs	4.73	1.03	1.36	57.0	3.04	36

The pseudopotential depends on two parameters: R_c and λ. The screening parameter λ is closely related to the Fermi wave vector k_F [8]:

$$\lambda^2 = \frac{4k_F}{\pi a_0} \tag{9}$$

where a_0 is the Bohr radius. The core radii R_c for alkali metals were estimated in [6] from fitting the experimental resistivities of liquid metals. We assume that they are the same the two-dimensional systems. The values of these parameters are also given in Table 1.

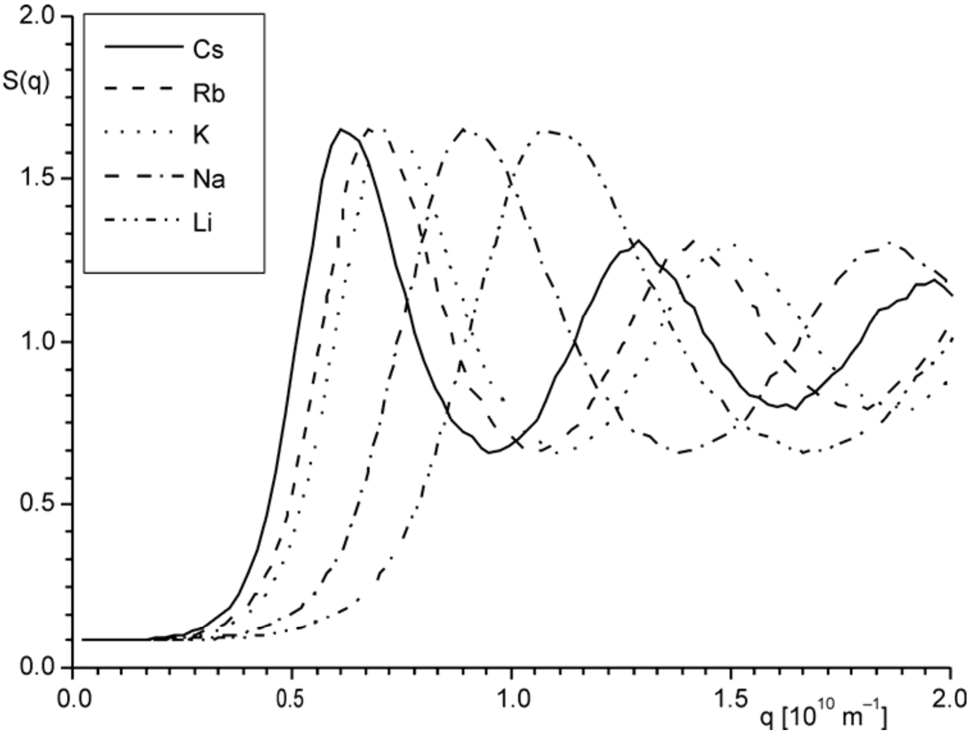

Fig. 1. Structure factors of alkali metals obtained from numerical simulations

The resistivities of the monolayer films of the considered metals, ρ_m, have been calculated by numerical integration and are shown in Table 1. It is interesting to compare the obtained values of ρ_m with the resistivities of the corresponding bulk materials, ρ_b. These quantities are measured in different units, so that when compare them we have to extrapolate our results to bulk values simply by multiplying them by the thickness of the layer, i. e. the atomic diameter. These results are also presented in Table 1, together with the experimental values for liquid metals.

4. Conclusions

We calculated the electrical resistivities of monatomic metallic layers, considering the transport of a two-dimensional electron gas through a disordered array of screened Shaw potentials. The resistivities obtained for alkali metals, after suitable extrapolation, are one order of magnitude smaller than the corresponding values for liquid metals. They are substantially lower because the electron in a two-dimensional system can be scattered only in a plane, whereas in a bulk material it has an additional degree of freedom. This means that these results can be viewed as reasonable, and could be confirmed by a suitable experiment.

References

[1] FARROW R.C., IBM J. Res. Develop., 42 (1998), 43.
[2] ŚLĘZAK T., KARAŚ W., KROP K., KUBIK M., WILGOCKA-ŚLĘZAK D., SPIRIDIS N., KORECKI J., J. Magn. Magn. Mater., 240 (2002), 362.
[3] ZIMAN J.M., Phil. Mag., 6 (1961), 1013.
[4] SPISAK B.J., PAJA A., Mol. Phys. Rep., 40 (2004), 144.
[5] SHAW Jr. R.W., Phys. Rev., 174 (1968), 769.
[6] JARGUZ P., PAJA A., to be published.
[7] ASHCROFT N.W., LEKNER J., Phys. Rev. 145 (1966), 83.
[8] ASHCROFT N.W., MERMIN N. D., Holt, Rinehart and Winston, New York, 1976.

Received 1 June 2005
Revised 10 October 2005