

# Conductivities and transmission coefficients of ultra-thin disordered metallic films

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The diffusive motion of quasi-two-dimensional electron gas through an ultra-thin system of disordered potentials is considered. In such a system, the Fermi sphere splits into a set of independent sheets due to a small thickness of the system. Each sheet can be seen as an electron subband. Electron transport goes through these subbands independently. The sum of electrical conductivities over the subbands determines the total current, which is calculated for ultra-thin films of cesium. We also present the relation between our approach and the Landauer formalism based on the notion of the transmission coefficient.

Key words: *electron transport; disorder; relaxation time; thin film; transmission coefficient*

## 1. Introduction

Low-dimensional systems are artificial structures very interesting for fundamental research, and on the other hand their potential applications in nanoscale technology bring about the rapid development of experimental techniques strongly supported by theoretical methods of analysing their electronic properties. One of the simplest examples of such a system is a thin film. In these structures, the motion of electrons is confined to a thin layer of metal or semiconductor. Motion perpendicular to the layer surface is frozen and the electrons compose a quasi-two-dimensional gas [1]. Size effects in the conductivity of ultra-thin films have been discussed by Fedorov et al. [2]. They considered crystalline films of Cu, composed of 1 to 32 monolayers. They took into account surface and impurity scattering, and assumed a random  $\delta$ -type impurity potential.

In our paper, we calculate the conductance of a totally disordered thin metallic film. We consider the scattering from all ionic potentials using the diffraction model for quasi-two-dimensional systems [3]. We neglect surface scattering, because we

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assume a planar motion of charge carriers. Moreover, we assume a realistic, Coulomb-screened potential, located at positions given by the structure factor. Our results are very close to those of Fedorov et al. [2].

## 2. Theoretical approaches to transport

As is well established, a proper quantum mechanical description of electron transport in disordered systems is based on the linearised von Neumann equation for the density matrix. In the lowest order of perturbation theory, the diagonal elements of the density matrix satisfy a Boltzmann-type equation [4]. This derivation is given for the case of randomly located potentials in metal. Additionally, it is assumed that atomic potentials have no internal structures, therefore electrons scatter from them elastically. The interaction between electrons and potentials is given by the collision integral  $I[f]$ , which can be modelled by the relaxation time approximation [5]

$$I[f] = -\frac{f(k) - f_0(k)}{\tau_{ir}} \quad (1)$$

where  $f(k)$  is a distribution function corresponding to small deviations from equilibrium as described by the Fermi–Dirac distribution function  $f_0(k)$ , and  $\tau_{ir}^{-1}$  is the inverse transport relaxation time.

Here we use the diffraction model proposed in our previous paper [3], where we put forward a scheme for calculating the inverse transport relaxation time in thin films. In this model, real atomic potentials are replaced by equivalent pseudopotentials that should give the same effect. In the considered case, the disorder in a thin film is characterized by a two-dimensional structure factor,  $S(q)$ , approximated by a parabola. Finally, the inverse transport relaxation time is given by the formula

$$\tau_{ir}^{-1} = \frac{1}{(2\pi)^2} \frac{m^*}{\hbar^3} \alpha u_0^2 \int_0^\pi d\varphi \frac{\sin^4 \frac{\varphi}{2}}{\frac{1}{\pi} \frac{1}{\alpha k_F} + \sin^2 \frac{\varphi}{2} \left[ 1 - \left( \frac{\pi m}{L_z k_F} \right)^2 \right]} \quad (2)$$

where  $\alpha$  is the prefactor of the parabola,  $u_0$  is the strength of the pseudopotential,  $L_z$  is the width of the layer in the  $z$ -direction, the number  $m = 1, 2, \dots$  is a subband index, and the remaining symbols have their usual meaning.

The formula given by Eq. (2) depends on the quantum number  $m$ . This can be simply explained, namely the finite thickness of the layer causes the Fermi sphere

split into a set of independent sheets. The electronic transport properties of each sheet are characterized by individual inverse transport relaxation times,  $[\tau_{tr}^{-1}]_m$ , and the number of electrons per unit area,  $n_m$ . The knowledge of these quantities allows us to calculate the inverse of resistivity or conductivity, which is given by the following formula [5]:

$$\sigma_m = \frac{1}{L_z} \frac{n_m e^2 \tau_m}{m^*} \quad (3)$$

where  $\tau_m$  is defined as the inverse of  $[\tau_{tr}^{-1}]_m$ .

As is well known, the Drude formula for the conductivity given by Eq. (3) can be derived from the semiclassical Boltzmann equation [6]. This expression, however, properly describes systems as far as  $k_F \ell \gg 1$ , where  $\ell$  is the mean free path. On the other hand, this condition determines the metallic regime, where the motion of electrons is diffusive. The total conductivity of a thin disordered metallic film in the present model is given by the formula

$$\sigma = \sum_{m=1}^{m_{\max}} \sigma_m \quad (4)$$

where  $m_{\max}$  is defined by condition (20) in Ref. [3].

Conductivity can be extracted from the conductance  $G$  as a function of layer thickness  $L_z$ , namely for a very thin stripe the conductance is given by the formula

$$G = \sigma(L_z) L_z \quad (5)$$

An alternative approach to the problem of electron transport in solids is based on the scattering properties of the system. Conductance in the linear transport regime is given by the formula [1,7]

$$G = \frac{2e^2}{h} \frac{T}{1-T} \quad (6)$$

where  $T$  is the total transmission coefficient.

If we substitute Eq. (3) into Eq. (4) and compare Eqs. (5) and (6), we obtain the total transmission coefficient in the following form:

$$T = \frac{\sum_{m=1}^{m_{\max}} \frac{n_m e^2 \tau_m}{m^*}}{\frac{2e^2}{h} + \sum_{m=1}^{m_{\max}} \frac{n_m e^2 \tau_m}{m^*}} \quad (7)$$

### 3. Numerical results

We performed calculations of total conductivity for a thin disordered film of cesium as a function of its thickness  $L_z$  using Eq. (4). The values of  $L_z$  taken for calculations corresponded to multiples of the atomic diameter of cesium. The Fermi vector for Cs was taken as  $k_F = 0.65 \times 10^{10} \text{ m}^{-1}$ , and the coefficient  $\alpha$  in the two-dimensional structure factor  $S(q)$  we equal to 0.28 after Ref. [8]. The results are presented in Fig. 1.

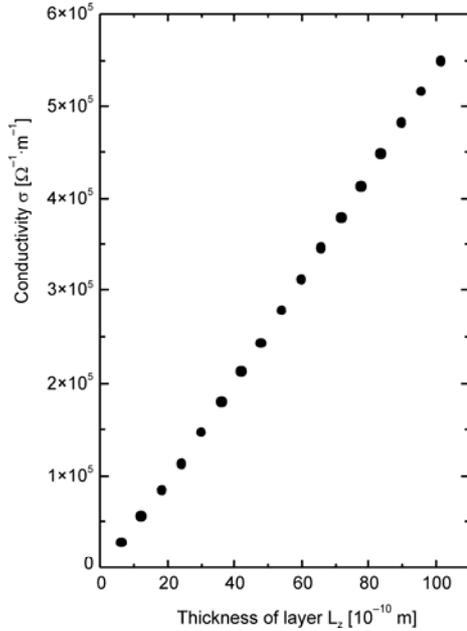


Fig. 1. Electrical conductivity of an ultra-thin film of Cs, calculated as a function of its thickness  $L_z$

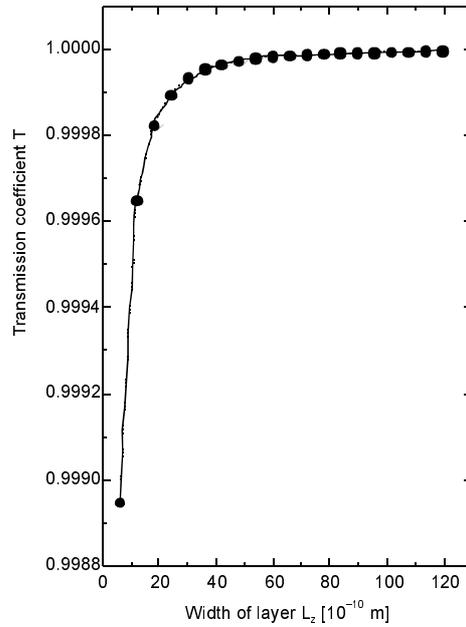


Fig. 2. Transmission coefficient of an ultra-thin film of Cs, calculated as a function of its thickness  $L_z$ . The solid line is a guide to the eye

The calculated conductivity  $\sigma$  increases almost linearly with increasing film thickness  $L_z$ . This is somewhat surprising, because  $\sigma$  is a material constant and should not depend on the size of the sample. In our model of quasi-two-dimensional electron gas, however, an increase of  $L_z$  gives rise to an increase of the number of open channels for electron transport. This is true if we neglect the transition between different electron subbands. If we take them into account, the inverse transport relaxation times become smaller and conductivity saturates. We can see that the transmission coefficient  $T$  actually saturates for  $L_z$  less than 100, which confirms our hypothesis about the conductivity.

### 4. Conclusions

We have used a diffraction model to investigate the electrical properties of a thin disordered metallic film, taking cesium as an example. We calculated the total con-

ductivity of a stripe with structural disorder for 1 to 17 monolayers as a function of its thickness. The dependence is monotonously increasing. The quantum size effect should be seen when integer multiples of half the Fermi wavelength fit exactly into the film thickness [9]. We calculated the conductivity for discrete values of the thickness (corresponding to full monolayers), and the deviations from monotonous behaviour occur between the points and cannot be seen.

Additionally, we find the relation between our model and a formalism based on the notion of the total transmission coefficient. The saturation observed in the transmission coefficient shows that electrical conductivity should also saturate in films that are thick enough.

In our approach, we do not discuss quantum interference effects between scattered electron waves, which lead to weak localization [9]. This is quite an important problem in two-dimensional systems, but on this level of approximation it can be justified, because only higher orders of perturbation theory for the density matrix include these effects [4, 10], and here we neglect these. We intend to incorporate these effects in future work.

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