Electron transport in disordered metallic nanosystems

A Paja
Faculty of Physics and Applied Computer Science,
AGH-University of Science and Technology, al. Mickiewicza 30, PL 30-059 Kraków, Poland

E-mail: paja@agh.edu.pl

Abstract. We consider the electron transport through a disordered metallic system, the size of which is less than 100 nm, at least in one dimension. We first present the main ideas of the theoretical description of the electron transport in bulk amorphous metals. Then we indicate the necessary modifications we should introduce to take into account the finite size of the considered sample. Finally, we discuss some examples of metallic nanostructures and calculate their electrical conductivity.

Introduction
The notion of nanosciences and nanotechnology appear in almost every branch of modern knowledge and technology. Heinrich Rohrer, the Nobel prize winner in 1986 (jointly with Gerd Binnig), clearly formulated the definition of the nanosciences [1]. According to his view, it is the science of dealing with nano-objects, i.e. manipulating, positioning and machining nano-objects, measuring, understanding and selectively modifying their properties as well as developing new concepts in treating them. I would only add that nanotechnology is the art of the fabrication of the nanosystems.

What do we call a “nanosystem”? As everybody knows, one nanometer equals to $10^{-9}$ m. The diameter of the smallest atom (hydrogen) is about $10^{-10}$ m, i. e. 0.1 nm. People agree that nano-objects (or nanosystems) are the assemblies of atoms the size of which is less than 100 nm, at least in one direction. Do we actually need a brand new theory for description of such objects? Yes and no. No, because we already have got a beautiful theory, quantum mechanics, which proved its usefulness even for smaller objects. On the other hand, if we want to apply the quantum theory of solid state to nanosystems we have to realize that almost all the results of this theory were obtained under the assumption that the size of a sample is large enough to treat the wave vector of electron as quasi-continuous variable. It is not true if the position of the electron is confined, at least in one dimension. Thus all previous calculations should be revised. The results, differing from those obtained for bulk materials, are called “quantum size-effects”. Also the considered systems gain new names: a cluster of atoms confined in each dimension is called “quantum dot”, a one-dimensional nanostructure is called “nanowire” and ultra-thin layer of atoms is treated as “quantum well”. In this work we will be dealing mainly with these last objects.

It is well known that the circuits of contemporary microelectronic devices are mostly made of semiconductors. The same is naturally foreseen for the oncoming nanoelectronics. The question

---

1 To whom any correspondence should be addressed.
arises why we are going to deal with metallic nanosystems. Single-electron transistors (SETs) are the nanodevices very important for investigation of fundamental physical phenomena as well as for applications. A very promising branch of electronics is spintronics, where the transport of the electron spin and charge are considered on equal footing. An essential feature of spintronics devices is that orientation of electron spin should be controlled over a length scale larger than the size of the device. The required orientation of spin is achieved by means of ferromagnetic leads and they are, of course, metallic.

A good example of such device is a ferromagnetic single-electron transistor (F-SET). It is well described in Ref. [2], therefore we mention here only some its features, essential for further considerations. The drain and source electrodes are made of a ferromagnetic metal and are connected to a central island by tunnel barriers. The requirement for the electrons to be well localised on the island is an appropriate resistance of the tunnel barriers. Moreover, the interplay between the Coulomb blockade in F-SETs and spin-dependent tunnelling processes gives rise to a novel phenomenon, enhanced tunnelling magnetoresistance (TMR). The value of TMR is defined as

$$\frac{R_{AP} - R_p}{R_p} = TMR$$

where $R_{AP}$ and $R_p$ are the device resistances in the antiparallel and parallel magnetisation configuration, respectively. It has been observed that the spin relaxation time can be enhanced by orders of magnitude as the size of the F-SET is reduced to a few nanometers [3]. A method of fabrication of nano-scale Ni/Au/Ni F-SET with a single 30 nm gold central island was presented in Ref. [2].

In view of above facts it is entirely justifiable to deal with electron transport properties of metallic nanosystems. Additionally, every real sample is actually disordered so that we have to consider the influence of disorder on the electrical conductivity of these nanosystems.

2. Theory of transport in disordered media

Every real sample of condensed matter is disordered. Nevertheless, we can imagine a perfectly ordered sample as our starting point for further considerations. It would be an infinite single crystal at the temperature $T=0$. The absolute zero is not available but we for the moment assume that it is possible. The deviations from the ideal crystal lattice at $T=0$ are called “static disorder”. They can take a form of isolated static defects (vacancies, foreign atoms, interstitial atoms, dislocations), or a chemical disorder visible in substitutional alloys, where different atoms occupy the sites of ideal lattice at random and, finally, a topological disorder in amorphous alloys (or metallic glasses) where atoms have got totally random positions. On the other hand, if we admit $T>0$ then a dynamic disorder appears. First of all, thermal vibrations of primarily perfect monoatomic lattice appear. The positions of atoms at a given moment of time are random, though they are close to their positions in perfectly ordered lattice. If the temperature reaches a definite for each solid value, $T_m$, each solid becomes a liquid (we neglect the possible effect of sublimation here). This way we move to the higher level of disorder, a topological one. If we assume that we have at least two types of atoms then we obtain a liquid alloy, the system which is disordered on the highest possible level, because it unifies both topological and chemical disorder.

The considerations on disorder are essential for our purpose: calculation of the conductivity (or resistivity) of real materials. We skip the problem of thermal vibrations in pure metals and the influence of isolated static defects on their resistivity because these subjects are treated in all textbooks on solid state physics. Calculation of the resistivity of substitutional alloys required quite new theoretical approach, the coherent potential approximation (CPA). This approach was originally proposed by Velicky et al. [4]. The main idea of this approach is the replacement of two real atomic potentials, $V_A$ and $V_B$, by one complex potential $\Sigma$. It is achieved by a simple assumption that the averaged scattering vanishes for this potential. The idea of CPA turned out very fruitful. Velicky [5] applied it to the problem of the electrical resistivity and obtained the Nordheim rule.
Mattis [6] extended the CPA method on partially ordered alloys and studied the order-disorder transition. Paja [7] calculated the electrical resistivity of partially ordered alloys as a function of their ordering parameter. Chen et al. [8] took into account the electron-phonon interaction in disordered alloys and showed that their resistivity could increase and decrease with temperature (or remain constant) in dependence on the strength of the electron-phonon coupling. This dependence is linear at low temperatures. It is suitable moment to say that the dependence of the resistivity on temperature in nanosystems may be quite different. In very thin (3 nm thick) disordered films of PdAu a logarithmic dependence is observed [9]. This dependence is of purely geometrical origin [10]. A dynamical theory of the resistivity of chemically disordered nanosystems is still waiting for its discoverer.

Much higher disorder appear in liquid and amorphous metals where no translational invariance is observed. The positions of atoms in space can be described only statistically, by means of the pair distribution function \( g(r) \) which determines the probability of finding an atom at the position \( r \) while the another atom is at the origin of the reference frame. The pair distribution function \( g(r) \) defined by

\[
\rho_0 \int_V g(r) d^3r = N
\]

is shown in Figure 1. Experimentally we can observe a structure factor \( S(q) \) which is related to \( g(r) \) by

\[
S(Q) = 1 + \rho_0 \int_V (g(r) - 1) \exp(-iQ \cdot r) d^3r
\]

and is shown in Figure 2.

![Figure 1](image1.png) **Figure 1.** Pair distribution function vs. distance between atoms .

![Figure 2](image2.png) **Figure 2.** Structure factor vs. the value of the wave vector.

Ziman [11] viewed the process of scattering electrons from the disordered array of atomic potentials as the diffraction of the electron wave on that array (the diffraction model). His formula for the electrical resistivity \( \rho \) of liquid metal reads

\[
\rho = \frac{3\pi m^2 \Omega_0}{4e^2 \hbar^3 k_F^6} \int_0^{2\pi} S(q) |U(q)|^2 q^3 dq
\]

where \( U(q) \) is the Fourier transform of the atomic potential, \( \Omega_0 \) is the atomic volume and other symbols have their usual meaning.

Faber and Ziman [12] extended the diffraction model onto liquid binary alloys. The description of the distribution of the positions of atoms requires three radial correlation functions \( g_{\alpha\beta}(r) \) thus the final formula for the resistivity exploits three partial structure factors \( S_{\alpha\beta}(q) \):
\[ \rho = \frac{3\pi m^2 \Omega_0}{4e^2 \hbar^2 k_F^6} \sum_{\alpha} \sum_{\beta} \left( c_{\alpha} c_{\beta} \right) \sqrt{S_{\alpha\beta}}(q) u_\alpha(q) u_\beta(q) Q^3 \, dq \]  

where \( c_\alpha \) and \( c_\beta \) are the atomic concentrations of the alloy components. The same formula applies for solid amorphous alloys due to similarity of liquid and amorphous structures.

3. Electron states in confined systems

In the standard quantum theory of the solid state we usually assume that the considered sample is infinite. The finite size of the sample is taken into account by the periodic boundary conditions and the wave vector of electron, \( k \), becomes a quasi-continuous variable. The dispersion relation in the free electron model

\[ E(k) = \frac{\hbar^2 k^2}{2m^*} \]  

(where \( m^* \) is the effective mass of the electron) allows us to define the Fermi surface

\[ \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2 k_z^2}{2m^*} = E_F \]  

and to calculate the electronic density of states

\[ D_3(E) = 2 \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E} \]  

For 2-dimensional electron gas the Fermi sphere degenerates into a circle

\[ \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} = E_F \]  

and the density of states becomes a constant [13]

\[ D_2(E) = 2 \frac{m^*}{2\pi \hbar^2} \]  

For 1-dimensional electron gas the Fermi surface reduces to 2 points

\[ k_x = \pm \sqrt{\frac{2m^* E_F}{\hbar}} \]  

and the density of states in this case reads

\[ D_1(E) = 2 \frac{\sqrt{2m^*}}{2\pi \hbar} \frac{1}{\sqrt{E}} \]

Let us consider now quasi-2-dimensional electron gas. It is a gas of electrons contained within a metallic film the thickness of which in the \( z \)-direction, \( L_z \), is less than 100 nm (Figure 3.). If the electron is free to move in \( x \) and \( y \) directions the Schrodinger equation for this case is

\[ \left( -\frac{\hbar^2}{2m^*} \Delta + V_{\text{conf}}(z) \right) \phi(r) = E \phi(r) \]
where the confining potential $V_{\text{conf}}(z)$ is illustrated in Figure 4.

![Diagram of thin film and confining potential](image)

**Figure 3.** Positioning of a thin film in a system of coordinates.

**Figure 4.** Confining potential along the $z$-axis.

The Equation (13) is easy to solve and its solution is

$$\phi_{k\rho}(\mathbf{r}) = \frac{1}{\sqrt{A}} \exp(i\mathbf{k}_\rho \mathbf{r}) \zeta_n(z)$$

(14)

where

$$\mathbf{r} = (x, y); \quad \mathbf{k}_\rho = (k_x, k_y); \quad A = L_x L_y$$

(15)

and

$$\zeta_n(z) = \sqrt{\frac{2}{L_z}} \sin \left( \frac{n\pi}{L_z} z \right)$$

(16)

The eigenvalues of energy are

$$\varepsilon_{kn} = \frac{\hbar^2 k^2}{2m^*} + \varepsilon_{zn}$$

(17)

where

$$\varepsilon_{zn} = \frac{\hbar^2}{2m^*} \left( \frac{n\pi}{L_z} \right)^2$$

(18)

Thus the Fermi sphere splits into a number of parallel sheets (Fig. 5)
The Fermi sphere separates into subbands. The following inequalities hold

$$\epsilon_{k_n} \leq E_F$$  \hspace{1cm} (19)$$

and

$$\frac{\hbar^2 k_n^2}{2m^*} \leq E_F - \epsilon_{k_n}$$  \hspace{1cm} (20)$$

The density of states changes into a function which is constant in subsequent intervals (“a staircase”).

**4. Electron transport in some specific disordered metallic nanosystems**

We consider a random array of scatterers represented by $S(q)$, embedded in the quantum well described above. The differential cross-section for in-plane scattering now is a function of a planar angle $\varphi$ only

$$\frac{d\sigma}{d\varphi} = \frac{1}{8\pi k_p} \left( \frac{m^*}{2\pi \hbar^2} \right)^2 N S(q) |u_s(q)|^2$$  \hspace{1cm} (21)$$

where

$$q = 2k_p \sin \frac{\varphi}{2}$$  \hspace{1cm} (22)$$

and $u_s(q)$ is a Fourier transform of a screened atomic potential $u_s(r)$.

The inverse transport relaxation time is

$$\frac{1}{\tau_{tr}} = 2\frac{v_F}{A} \int_0^\pi d\varphi \frac{d\sigma}{d\varphi} (1-\cos \varphi)$$  \hspace{1cm} (23)$$

Equations (22) and (23) allow us for calculation of the resistivity $\rho_n$ for the $n$-th subband.
\[ \rho_n = \frac{m^*}{n_e^2 \tau_{tr}} \]  

(24)

where \( n_c \) is the area concentration of carriers, because both \( k_p \) and \( n_c \) depend on the subband. The total Drude conductivity is a sum over all subbands

\[ \sigma_D = \sum_{n=1}^{n_{\text{max}}} \sigma_n = \sum_{n=1}^{n_{\text{max}}} \frac{1}{\rho_n} \]  

(25)

4.1. Electrical resistivity of ultrathin disordered metallic film

We at first considered the transport of exactly 2-D electron gas through a disordered array of screened Shaw pseudopotentials [14]. We assumed an alkali monoatomic amorphous film for calculations \((n=1)\). The structure factor was obtained by means of numerical simulation. It turned out to be very similar to that of for 3-D case. The results of our calculations for five alkali metals are presented in the Table 1.

Table 1. Resistivities of alkali metals calculated for the monolayer films in comparison with the experimental values for bulk metals.

| Element | Diameter of the hard sphere \( \sigma \) \[10^{-10} \text{ m}\] | Screening parameter \( \lambda \) \[10^{10} \text{ m}\] | Core radius \( R_c \) \[10^{-10} \text{ m}\] | Resistivity of monolayer \( \rho_m \) \[\mu\Omega \text{ cm}\] | Experimental bulk resistivity \( \rho_{\text{exp}} \) \[\mu\Omega \text{ cm}\] |
|---------|------------------|-------------------|------------------|------------------|------------------|
| Li      | 2.70             | 1.36              | 0.66             | 55.4             | 25               |
| Na      | 3.28             | 1.23              | 1.25             | 19.7             | 9.6              |
| K       | 4.07             | 1.11              | 1.53             | 22.2             | 13               |
| Rb      | 4.30             | 1.08              | 1.47             | 31.8             | 22               |
| Cs      | 4.73             | 1.03              | 1.36             | 57.0             | 36               |

As we can see the resistivity of the monolayer is in each case higher than the experimental value for the bulk material (i.e. the conductivity is lower).

We next tested our model for films consisted of more than one monolayer [15]. We showed that the conductivity increases with the thickness of the film (see Figure 6).
The conductivity should saturate as we move to bulk samples. Indeed, we have shown that in our next work.

4.2. Spin scattering of conduction electrons in quasi-two-dimensional system

We assume the current of polarised electrons going through a disordered array of $N_A$ non-magnetic atoms doped with $N_B$ magnetic impurities, placed at random [16]. Let spins of conduction electrons and impurities be polarised along the $z$-axis and in the same direction. The Hamiltonian of the conduction electron reads

$$
\hat{H} = -\frac{\hbar^2}{2m^*} \Delta + U_0(p) + U_{ss}(p) 
$$

(26)

where the atomic potential

$$
U_0(p) = \sum_{j=1}^{N_A} u_{aa}(p - R_j) + \sum_{j=1}^{N_B} u_{ah}(p - R_j) 
$$

(27)

and the exchange potential

$$
U_{ss}(p) = -\sum_{j=1}^{N_B} J_s \delta(p - R_j) s_z(p) S_z(R_j) 
$$

(28)

The total differential cross-section is

$$
\frac{d\sigma}{d\varphi} = \frac{d\sigma_0^A}{d\varphi} + \frac{d\sigma_0^B}{d\varphi} + \frac{d\sigma_{1\uparrow}}{d\varphi} 
$$

(29)
where the atomic part is
\[
\frac{d\sigma_0^X}{d\varphi} = \frac{1}{8\pi k_\rho} \left( \frac{m^*}{2\pi \hbar^2} \right)^2 N_X S_X(q) |u_{aX}(q)|^2, \quad X = A, B
\]
(30) and the spin part
\[
\frac{d\sigma^B_\uparrow \downarrow}{d\varphi} = \frac{1}{8\pi k_\rho} \left( \frac{m^* J_0}{2\pi \hbar^2} \right)^2 S(S+1) N^2 B S_B(q)
\]
(31) We assumed here the Coulomb screened potential
\[
u_{aX}(\rho) = u_X \frac{\exp(-\lambda_X \rho)}{\rho}
\]
(32) then its Fourier transform is
\[
u_{aX}(q) = 2\pi u_X \frac{1}{\sqrt{\lambda^2_X + q^2}}
\]
(33) We approximated the structure factor by a parabola
\[
S_X(q) \approx \alpha_X q^2
\]
(34) which is a good approximation in the range $[0, 2k_F]$. The conductivity of the $m$-th sheet of the Fermi surface
\[
\sigma_m(L_z, x) = \frac{1}{L_z} \frac{n_\rho e^2 \tau_m}{m^*}
\]
(35) depends on $L_z$ and the concentration $x = N_B/(N_A + N_B)$ of magnetic impurities. The dependence of $\sigma_m$ on $L_z$ is through $k_\rho$ which is different for either sheet
\[
k_\rho = \sqrt{\frac{2m^* E_F}{\hbar^2} - \left( \frac{m \pi}{L_z} \right)^2}
\]
(36) The total conductivity of the considered film is
\[
\sigma_{tot}(L_z, x) = \sum_{m=1}^{m_{max}} \sigma_m(L_z, x)
\]
(37) where $m_{max}$ also depends on the system size $L_z$.

The results of calculations for the conductivity $\sigma$ as a function of the film thickness $L_z$ are shown in Figure 7, and as the function of concentration of magnetic impurities $x$ in Figure 8.

**Figure 7.** The conductivity $\sigma$ as a function of the film thickness $L_z$ for the concentration of magnetic impurities $x=0.05$

**Figure 8.** The conductivity $\sigma$ as a function of concentration of magnetic impurities $x$
It is clear that the conductivity saturates for the film thickness greater than 100 monolayers.

4.3. Conductivity of a disordered magnetic monoatomic layer.

We considered a 2-D disorder array of magnetic atoms. We assume the spins can have only one of two possible orientations: “up” and “down.” Thus the system can be treated as a 2-component disordered magnetic alloy [17]. Let the current go along the magnetisation axis. It can serve as an axis of quantazition. Each electron in the current takes one of the two possible orientations of its spin: parallel and antiparallel to magnetisation. There is well-known asymmetry of scattering in this case: electrons with spins parallel to that of scatterer feel only the Coulomb potential whereas those having opposite spins scatter more strongly [18].

We assume the total scattering potential

\[ U(r) = U_1(p) + U_2(z) \]  

where

\[ U_1(p) = \sum_{i=1}^{N} u_s(p - R_i) u_s(R_i) \]  

\[ U_2(z) \] is the geometrical confinement and \( u_s(R_i) \) is the spin part of atomic potential. The electron wave function has the form

\[ \psi_s(r) = \phi(p) \zeta(z) \chi(s), \quad s = \pm 1 \]

We now can define the operator \( u_s(R_i) \) by its matrix elements

\[ \chi(s) u_s(R_i) \chi(s') = \delta_{ss'} (t + (1-t) \delta_{Nz}), \quad t \geq 1 \]

This definition assures us that the scattering in case of opposite spins is \( t \) times stronger. Thus the transport relaxation times for “spin-up” and “spin-down” differ substantially:

\[ \frac{1}{\tau_u} = \frac{1}{4\pi k_p} \left( \frac{m}{2\pi h^2} \right)^2 \int_0^\pi d\phi \left( 1 - \cos \phi \right) u^2_s(q) \left[ c_1 S_1(q) + 2(c_1c_2)\sqrt{2} S_{12}(q) + c_2 S_{22}(q) \right] \]  

\[ \frac{1}{\tau_d} = \frac{1}{4\pi k_p} \left( \frac{m}{2\pi h^2} \right)^2 \int_0^\pi d\phi \left( 1 - \cos \phi \right) u^2_s(q) \left[ c_1^2 S_1(q) + 2(c_1c_2)\sqrt{2} S_{12}(q) + c_2 S_{22}(q) \right] \]

where \( c_1 \) and \( c_2 \) are the fractions of atoms polarised “up” and “down” which can be expressed by magnetisation \( \mu \)

\[ c_1 = \frac{1 + \mu}{2}, \quad c_2 = \frac{1 - \mu}{2} \]

The conductivities \( \sigma^+ \) and \( \sigma^- \) are given by

\[ \sigma^\pm = \frac{n_e e^2 \tau^\pm_{\mu}}{m L_z} \]

and the total conductivity in two-band model

\[ \sigma_{tot} = \sigma^+ + \sigma^- \]

The results calculated for some model set of parameters are shown in Figure 9.
We can see that for asymmetry parameter $t=1$ the conductivity is constant as expected and for higher values of $t$ the conductivity rises rapidly as the relative magnetisation $\mu$ approaches unity.

5. Summary

Contemporary electronics is based on circuits made of semiconducting materials. Most electronic devices exploit the transportation of the electron charge. Spintronics is a new branch of electronics which is going to manipulate the electron spin as well. Metallic nanosystems are important both for study of the behaviour of spin in the nanoscale as well as for applications. But real metallic nanosystems are disordered in most cases. In this work some specific metallic nanosystems were studied by means of methods developed for bulk disordered samples. It has been shown that the transport coefficients of such nanosystems depend on their size and differ substantially from the values for bulk materials but they approach the bulk values when their size reaches about a hundred monoatomic layers.

Acknowledgements

The author thanks dr. B. J. Spisak, Mr. P. Jarguz, MSc. Eng., and Mr. M. Ornat, MSc. Eng. for fruitful collaboration.
References

[1] Rohrer H 1996 Microelectron. Eng. 32 5
[2] Yakushiji K, Ernult F, Imamura H, Yamana K, Mitani S, Takanashi K, Takahashi S, Maekawa S and Fujimori H 2005 Nature Materials 4 57
[3] Petterson H, Liu R, Suyatin D and Samuelson L 2008 Assembling F-SET with AFM Nanostructures in Electronics and Photonics ed F Rahman (Singapore: Pan Stanford Publishing) chapter 2 pp 29-40
[4] Velicky B, Kirkpatrick S and Ehrenreich H 1968 Phys. Rev. 175 747
[5] Velicky B 1969 Phys. Rev. 184 614
[6] Plischke M and Mattis D 1973 Phys. Rev. B 7 2430
[7] Paja A 1976 J. Phys. C: Solid State Phys. 9 1445
[8] Chen A B, Weisz G and Sher A 1972 Phys. Rev. B 5 2897
[9] Dolan G J and Osheroff D D 1979 Phys. Rev. Lett. 43 721
[10] Akkermans E and Montambaux G 2007 Mesoscopic Physics of Electrons and Photons (Cambridge: Cambridge University Press)
[11] Ziman J M 1961 Phil. Mag. 6 1013
[12] Faber T E and Ziman J M 1965 Phil. Mag. 11 153
[13] Heinzel T 2007 Mesoscopic Electronics in Solid State Nanostructures (Weinheim: WILEY-VCH Verlag GmbH&Co. KgaA)
[14] Jarguz P and Paja A 2006 Mat. Sci. – Poland 24 633
[15] Spisak B J and Paja A 2006 Mat. Sci. – Poland 24 605
[16] Paja A and Spisak B J 2007 Acta Phys. Pol. A 112 1289
[17] Paja A and Spisak B J 2008 Mat. Sci. – Poland 26 1009
[18] Camley R E and Barnas J 1989 Phys. Rev. Lett. 63 664