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Electron mean free path model for rectangular nanowire, nanofilm and nanoparticle

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ABSTRACT

With the top-surface scattering considered, an improved model was proposed in this paper to predict the electron mean free path (EMFP) of a rectangular nanowire. The proposal of this model was based on the statistic simulation and the related fittings. The model is generally suitable for predicting EMFPs of rectangular nanowires, nanofilms and nanoparticles. The top-surface scattering was studied based on the model. And some issues about the Cu rectangular nanowires, rather than the widely studied sidewall-surface scattering and the grain-boundary scattering, were discussed. It is predicted that the top-surface scattering would be important if the length of the nanowire is close to the size of the cross-section. If short nanowires, with the same cross-sectional area but different lengths, are prepared and tested, the effect of top-surface scattering may be observable. Though a good resistivity agreement between the model and the experiment can be reached, fitting parameters of the model may be quite different for different authors, even with the same nanowire considered.

1. Introduction

With electronic-device size decreasing to nanoscale, the electronic thermal conductivity and the electrical conductivity of nanowire and nanofilm have drawn considerable attention. The surface scattering and the grain-boundary scattering, as the main contributions to the size effect of electron mean free path (EMFP), have been the subject of intense research for decades. The widely accepted Fuchs–Sondheimer (FS) model [1,2] and the Mayadas–Shatzkes (MS) model [3] have been separately developed to describe the sidewall-surface scattering and the grain-boundary scattering. Following Matthiessen's rule, the combined model could be obtained and described as the FS–MS model [4].

The FS model [1,2] with just sidewall-surface scattering considered was described as

$$\rho_{FS}=\rho_0\left[1+\frac{3}{8}l_0(1-p)\left(\frac{1}{t}+\frac{1}{w}\right)\right], \tag{1}$$

where ρ_{FS} and ρ_0 are electrical resistivities of the nanowire and the corresponding bulk, respectively, l_0 is the bulk EMFP at some temperature, and t and w are the thickness and the width of the nanowire, respectively. p is the specular coefficient signifying the ratio of the specular scattering to the total scattering.

In addition to the surface scattering, while the nanostructure may be not single crystal but polycrystalline, the grain-boundary scattering was taken into account by the MS model [3], expressed as

$$\rho_{MS}=\rho_0\left[1-\frac{3}{2}\alpha+3\alpha^2-3\alpha^3\ln\left(1+\frac{1}{\alpha}\right)\right]^{-1}, \tag{2}$$

where $\alpha=(l_0/D)R/(1-R)$, D is the average grain size, R is the reflection coefficient, signifying the fraction of electrons that are not scattered by the potential barrier at a grain boundary. Under the condition of small α, Eq. (2) can be simplified as [3]

$$\rho_{MS}=\rho_0\left[1+\left(\frac{3}{2}\right)\left(\frac{l_0}{D}\right)\left(\frac{R}{1-R}\right)\right]. \tag{3}$$

For common case $\alpha\leq 0.5$, the deviation of Eq. (3) from Eq. (2) is less than 3%. Based on the FS model or the MS model, the corresponding EMFP l can be further obtained by the widely accepted relation, $\rho l=mv/(ne^2)=$constant, [5–7] which can be derived from $\sigma=ne^2l/(mv)$ and $\rho=1/\sigma$, [8] where σ is the electrical conductivity, n is the number of electrons per unit volume, e is the electron charge, m is the mass of a free electron, and v is the electron velocity.

While the sidewall-surface scattering and the grain-boundary scattering have already been considered by the FS model and the MS model, the present paper was aimed to further consider the top-surface scattering into account through a theoretical approach.

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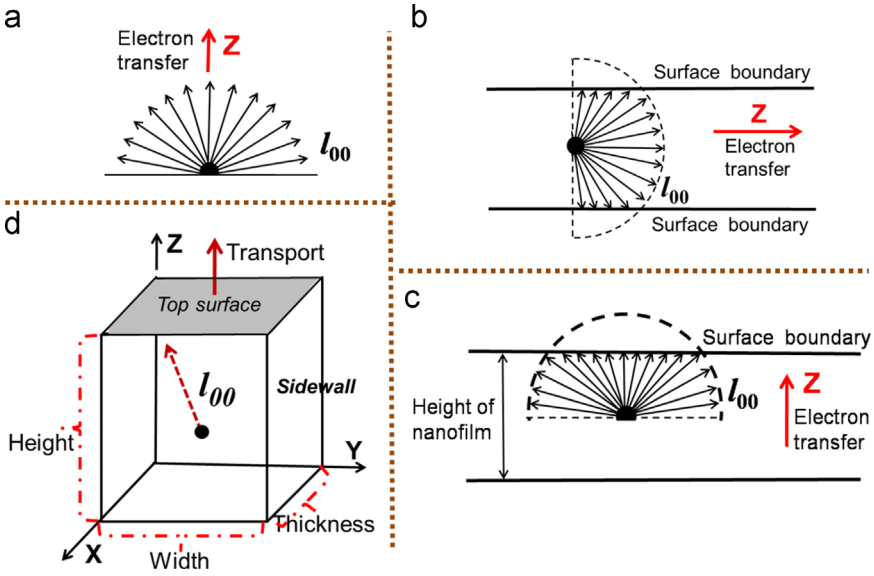

Fig. 1. Schematic EMFP distributions: (a) in the metallic bulk, (b) along the in-plane direction in the nanofilm and (c) along the cross-plane direction in the nanofilm, (d) 3D simulation domain.

The top-surface means the interface through which electrons transport from one structure to another, as shown in Fig. 1(d). Actually, the theoretical approach, combining geometric arguments with kinetic theory, has already been widely applied to examine the size effect of the sidewall-surface scattering on the electron transfer in different structures, such as high-Tc superconductors, [9] thin wires with circular and rectangular cross-sections [10–12], Cu and Au nanofilms [13], etc. And an extensive review has already been given by Iniewski [14].

Since the theoretical method is mathematically cumbersome, an alternative statistical simulation method, which is based on the geometric arguments, was setup and performed in this paper; subsequently, a fitting formula based on the simulation results was proposed to consider the top-surface scattering. Since there is still no available experiments to consider the top-surface scattering, the top-surface scattering was only discussed based on the model. Concerning the sidewall-surface scattering and the grain-boundary scattering, some experimental resistivities of Cu rectangular nanowires were compared and analyzed. Considering that the size effect of either electronic thermal conductivity or electrical resistivity directly attributes to the restrictions of the EMFP [9,15], only the EMFP was discussed in this paper. Of course, the EMFP result can be further applied to calculate the electronic thermal conductivity and the electrical resistivity.

2. Methodology

2.1. Simulation method

Before the introduction of the simulation method, the transport of electrons in the metallic bulk should be illustrated first. For the analysis, the net electron transfer was assumed to be along the Z direction, and the perpendicular plane was the XY plane, as shown in Fig. 1(a). In a metallic bulk, electrons will transfer with equal likelihood in all directions along the positive Z direction with a free path, l_{00}, as illustrated in Fig. 1(a). Then the bulk EMFP, l_0, which is the average positive-Z-direction component of all possible l_{00} over the hemisphere, can be calculated as

$$l_0 = \frac{\int_0^{2\pi} d\varphi \int_0^{\pi/2} l_{00} \cos(\theta) d\theta}{\int_0^{2\pi} d\varphi \int_0^{\pi/2} d\theta} = \frac{2}{\pi} l_{00}, \tag{4}$$

where θ is the angle between the electron transport direction and the Z axis, φ is the angle between the projection of the electron-transport direction in the XY plane and the positive X axis. Since the bulk value of l_0 is available for most metals, l_{00} can be obtained by Eq. (4) and further applied in the simulation.

Then, a kind of statistical simulation method for calculating the EMFP considering only surface scattering was setup. In the simulation, the following hypotheses were applied: (a) independent electrons are randomly distributed in the nanomaterial; (b) each electron moves along a straight line with the Fermi velocity until terminated at the boundary or long enough path (l_{00}) has been traveled, and only the Z component of l_{00} contributes to the EMFP; (c) the electron-surface scattering was totally inelastic or diffuse [9]. The simulation process is shown in Fig. 2.

Employing the statistical simulation method, the totally diffuse EMFP, l_1, can be obtained. With l_1 obtained, by introducing the specular coefficient p, we can further take the specular or elastic scattering into account based on the Matthiessen rule [8] with the following expression:

$$\frac{1}{l} = p\frac{1}{l_0} + (1-p)\frac{1}{l_1}. \tag{5}$$

In fact, Eq. (5) is also the rule for FS model to include the specular scattering effect.

To validate the simulation method, the simulated totally-diffuse EMFP l_1 of Cu square nanowires is shown in Fig. 3. And the simulation result was further compared with results predicted both by FS model ($p=0$) and by Boltzmann transport equation (BTE) [16]. All results were scaled by the Cu bulk EMFP ($l_0=39$ nm) [17]. It was shown that there are good agreements between different methods. Deviation of our statistical simulation result from that of the FS model is less than 5%.

2.2. Model proposal

To consider the top-surface scattering (height size effect), the transport along the height of the Cu nanofilm (or along the cross-plane direction) was considered, where the sidewall-surface scattering can be omitted, as shown in Fig. 1(c). An expression similar to the FS model was proposed to figure out the top-surface