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Influence of surface roughness on the electrical conductivity of semiconducting thin films

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HIGHLIGHTS

- The Green function solution of the Boltzmann transport equation has been applied.
- σ_{xx} increases with increasing l for Gaussian and exponential models.
- σ_{xx} values are in the same order as the other two models for the power law model.
- Our results provide the equation $\sigma \sim L^6$ with L the film thickness.
- Our results are well consistent with the ones obtained by other methods.

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ABSTRACT

The Green function solution of the Boltzmann transport equation has been applied in case of no magnetic field by ignoring any volume impurities. Gaussian, exponential and power law models for the surface roughness correlation function have been studied and the results have been compared with the ones obtained by other methods. It has been found that the electrical conductivity σ increases with increasing correlation length l for the first two models, while for the third model σ value is of the same order as the first two models. Therefore we show that the shape of the surface roughness can strongly influence the electrical properties.

1. Introduction

The effects of boundary scattering on transport processes is a topic of broad interest because of the fundamental and technological importance in microelectronic devices [1–9], wires, wells and thin films [10], semiconductor industry [11] and nanofabrication. The technical importance of scattering from rough surfaces has attracted the attention of researchers and many papers about this issue have been published in recent years [12–20]. The miniaturization effort in the electronic industry has required better understanding of additional charge scattering by rough surfaces [21]. Boundary scattering is especially important for transport in ultrathin and/or clean systems in which the particle mean free path is comparable to the system size [8]. Therefore the effects of surface roughness parameters on electrical conductivity have to be taken into account carefully in explaining electrical transport properties.

Surface inhomogeneities in semiconducting thin films influence the electrical conductivity because of additional charge scattering [9,22–37]. For a film with a smooth surface, increment of the film thickness L leads to higher film conductivity. However the development of boundary roughness which may be inevitable during the increase of the thickness, reduces the

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conductivity due to boundary scattering, and causes an adverse effect. It is generally agreed that the electrical conductivity of semiconducting thin films, limited by roughness scattering, follows a power law $\sigma \propto L^6$ [1–3]. In this theoretical work for simplicity, the surface roughness is assumed to be constant with thickness.

In a previous paper [38] we have studied the effects of boundary roughness on the electrical conductivity of semiconducting thin films under no magnetic field. In that study we used a finite relaxation time τ_0, which results from scattering by impurities, grain boundaries and defects in the system in the absence of roughness effects. In this study we use an infinite τ_0 and consider only the contribution from the surface roughness and disregard bulk scattering. We have shown how to calculate the electrical conductivity of a semiconducting thin film with rough boundaries and how the surface of the structure affects the electrical transport by the Green function solution method of the Boltzmann transport equation. The developed method is a simple and general solution which can be easily applied to semiconducting thin films with rough boundaries for different types of magnetic field and relaxation times. In this framework we have studied the dependence of longitudinal conductivity on the shape of the correlation function in detail and compared our results with the ones which were calculated by the Golden rule based method. We have also compared the theoretical L dependence of σ with the experimental curve.

In Section 2 the model is introduced and surface roughness correlation functions are given. In Section 3 the Green function solution method of Boltzmann transport equation is given briefly. Section 4 is about comparison of σ with other theoretical studies for three different types of correlation functions, where a comparison of σ vs L curve for an experimental study is also given. Section 5 contains the conclusions.

2. Correlation function

An ideal two-dimensional (2D) film with perfect smooth surfaces perpendicular to the z axis is defined by the equations $z = \pm L/2$ with L the average film thickness. If both surfaces of the film are rough, the boundaries are $z = \pm L/2 \mp \xi(\boldsymbol{r})$. Here, $\xi(\boldsymbol{r})$ are the random roughness fluctuations which are assumed to be single-valued functions of the in-plane vector $\boldsymbol{r} = (x, y)$. The boundary inhomogeneities are small, $\xi(\boldsymbol{r}) \ll L$, and random with zero average $\langle\xi\rangle = 0$. The calculations are performed with the help of a coordinate transformation which reduces a transport problem with rough random walls to an equivalent problem with ideal smooth walls [10]. Then, in new coordinates, the transformed bulk Hamiltonian contains a random potential energy term $V(\boldsymbol{r})$:

$$V(\boldsymbol{r}) = \sum_{i=1}^{N} V_1(\boldsymbol{r} - \boldsymbol{R}_i) = \left(\frac{\pi\hbar j}{L}\right)^2 \frac{\xi(\boldsymbol{r})}{mL}. \tag{1}$$

The random potential energy $V(\boldsymbol{r})$ is the sum of $V_1(\boldsymbol{r} - \boldsymbol{R}_i)$ individual potential functions which are situated at random $\boldsymbol{R}_i$ positions on the surface. The random potential energy which is contained as a perturbation term in the transformed Hamiltonian causes a random electrical potential $\phi_p = V(\boldsymbol{r})/e$, a random electrical field $\boldsymbol{E}_1 = -\nabla\phi_p$ and a spatial variation of the Fermi velocity $\nabla\delta v(\boldsymbol{r}) = V(\boldsymbol{r})/P_F = \sum_i v_1(\boldsymbol{r} - \boldsymbol{R}_i)$ [39] where P_F is the Fermi momentum. We get the variation of the Fermi velocity by the equation $\frac{1}{2}m\,[v_F + \delta v(\boldsymbol{r})]^2 = E_F + V(\boldsymbol{r})$.

The form of the roughness correlation function plays a significant role on the electrical conductivity. Surface roughness and/or thickness fluctuation is characterized by a correlation function which has different notations for different shapes. The surface roughness correlation function contains parameters related to the magnitude of the system. The main characteristics of the surface correlation function are the rms roughness amplitude Δ, the in-plane roughness correlation length l and the roughness exponent H. l is a measure of the average distance between peaks and valleys on the surface. The roughness exponent $0 \le H \le 1$ is a degree of surface irregularity [40–42]. Large values of H corresponds to smoother height–height fluctuations. The effects of H were shown to have a significant influence on the conductivity for both metallic and semiconducting films [4,43]. Among the three surface roughness parameters (Δ, l and H), the main interplay of the roughness effect occurs for H and l. The parameter Δ has a trivial effect on the conductivity because of the form $\sigma \sim \Delta^{-2}$ [4].

While $F(\rho) = \overline{V(\boldsymbol{r})V(\boldsymbol{r}')} = \frac{1}{A}\int V(\boldsymbol{\rho} + \boldsymbol{R})V(\boldsymbol{R})\mathrm{d}^2\boldsymbol{R}$ shows the random potential correlation function, $f(\rho) = \overline{\xi(\boldsymbol{r})\xi(\boldsymbol{r}')}$ shows the surface roughness correlation function in real space. The roughness is assumed isotropic, so the correlation functions depend only on the relative distance $\rho = |\boldsymbol{r} - \boldsymbol{r}'|$. The random potential correlation function in real space is defined in the following where the overbar shows configuration averaging:

$$F(\rho) = \overline{V(\boldsymbol{r})V(\boldsymbol{r}')} = \left(\frac{\pi\hbar}{L}\right)^4 \frac{\overline{\xi(\boldsymbol{r})\xi(\boldsymbol{r}')}}{m^2L^2} = \left(\frac{\pi\hbar}{L}\right)^4 \frac{f(\rho)}{m^2L^2}. \tag{2}$$

Several shapes can be used for $F(\rho)$ or its Fourier transform $\widetilde{F}(k)$ for surface inhomogeneities. While Gaussian model $F(\rho) \sim \mathrm{e}^{-\rho^2/l^2}$ is commonly used in theoretical applications, exponential model $F(\rho) \sim \mathrm{e}^{-\rho/l}$ provides a better fit to experimental data [8]. A third model is [44] provided by the power law correlation function $F(\rho) \sim \rho^{\alpha}$. In this study the dependence of longitudinal conductivity on the correlation length for different parameters will be studied for the two main models of the correlation function. The third model has no correlation length l but gives σ values in the range of the previous two provided we use the same values for Δ and the volume electron density c and we provide a σ vs L curve for it.