Microelectronic Engineering 167 (2017) 37–41

Contents lists available at ScienceDirect

Microelectronic Engineering

journal homepage: www.elsevier.com/locate/mee

Research paper

Resistivity scaling in metallic thin films and nanowires due to grain boundary and surface roughness scattering

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ARTICLE INFO

Article history:
Received 29 April 2016
Received in revised form 8 October 2016
Accepted 17 October 2016
Available online 20 October 2016

Keywords:
Resistivity scaling
Surface roughness
Grain boundaries
Electron scattering
Electron transport
Nanowires
Thin films
Semiclassical Boltzmann equation
Fermi's golden rule

ABSTRACT

A modeling approach, based on an analytical solution of the semiclassical multi-subband Boltzmann transport equation, is presented to study resistivity scaling in metallic thin films and nanowires due to grain boundary and surface roughness scattering. While taking into account the detailed statistical properties of grains, roughness and barrier material as well as the metallic band structure and quantum mechanical aspects of scattering and confinement, the model does not rely on phenomenological fitting parameters.

1. Introduction

The resistivity of metallic thin films and nanowires increases drastically when the film thickness or wire diameter is reduced [1]. An increased resistivity is undesirable for typical applications of these structures, e.g. interconnects in semiconductor devices, as it leads to increased heating, power dissipation, signal propagation delays, etc. Hence, in order to assess the performance of metallic thin films and nanowires as conductors in nanoscaled applications, it is important to study their resistivity and scaling behavior and understand how a drastic increase of resistivity can be prevented, if at all possible for metallic structures with sub-10 nm dimensions.

Experimental data has indicated that the increase of resistivity is mainly induced by an increase of electron scattering at the grain boundaries and near the rough boundaries of the structure. These scattering mechanisms lead to a resistivity contribution that adds to the bulk resistivity dominated by the electron-phonon interaction and scattering with lattice imperfections which is, to a good approximation, independent of the thickness. The resistivity data of metallic thin films and wires is in good agreement with the semiclassical Mayadas-Shatzkes model, commonly used for data comparison and predicting a resistivity scaling almost inversely proportional to the film width or wire diameter [1,2]. While the Mayadas-Shatzkes model provides satisfactory fits to the data, it contains phenomenological fitting parameters: a specularity parameter for boundary surface scattering and a reflection coefficient for grain boundary scattering. These parameters do not provide a clear connection between the microscopic scattering events and the resulting, measured resistivity of the thin film or nanowire. For example, there is no clear relation between boundary roughness, the microscopic origin of diffusive scattering at the boundary, and the phenomenological specularity parameter in the Mayadas-Shatzkes model which intends to capture this process. Moreover, the Mayadas-Shatzkes model neglects the material band structure properties and quantum mechanical aspects of scattering and confinement while a priori there is no reason to expect that both aspects have negligible impact on the resistivity scaling behavior.

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http://dx.doi.org/10.1016/j.mee.2016.10.015
0167-9317/

We present an alternative approach to model resistivity scaling in metallic thin films and nanowires, based on the multi-subband Boltzmann transport equation, with averaged scattering rates obtained from Fermi's golden rule for grain boundary and surface roughness scattering [3,4]. Our approach allows to perform a rigorous analysis of the resistivity and its scaling behavior while taking into account the aforementioned aspects that are neglected in some conventional approaches.

In Section 2 we summarize briefly the theory of the semiclassical multi-subband Boltzmann equation and the scattering rates obtained with Fermi's golden rule for grain boundary and surface roughness scattering. Next, we present some simulation results in Section 3, which are discussed in Section 4, followed by a conclusion in Section 5. We also refer to some articles with similar developments for metallic thin films and nanowires [5–7].

2. Theory

The electron (or hole) transport formalism based on the semiclassical multi-subband Boltzmann transport equation can be summarized by the following list of equations:

$$\mathbf{J} = \sum_{\mathbf{n}} \int \frac{\mathrm{d}^D k}{(2\pi)^D} \, \frac{q \, \nabla_{\mathbf{k}} E_{\mathbf{n}}(\mathbf{k})}{\hbar} \, \delta f_{\mathbf{n}}(\mathbf{k}), \tag{1}$$

$$\delta f_{\mathbf{n}}(\mathbf{k}) = \frac{q \, \mathbf{E} \cdot \nabla_{\mathbf{k}} E_{\mathbf{n}}(\mathbf{k})}{\hbar} \, \tau_{\mathbf{n}}(\mathbf{k}) \, \delta \left(E_{\mathbf{n}}(\mathbf{k}) - E_{\mathrm{F}} \right), \tag{2}$$

$$\frac{1}{\tau_{\mathbf{n}}(\mathbf{k})} = \sum_{\mathbf{n}',\mathbf{k}'} \left(1 - \frac{\tau_{\mathbf{n}'}(\mathbf{k}') \, \partial_{k'} E_{\mathbf{n}'}(\mathbf{k}')}{\tau_{\mathbf{n}}(\mathbf{k}) \, \partial_k E_{\mathbf{n}}(\mathbf{k})} \right) P\left(|\mathbf{n} \; \mathbf{k}\rangle \rightarrow |\mathbf{n}' \; \mathbf{k}'\rangle \right), \tag{3}$$

$$P\left(|i\rangle \rightarrow |f\rangle \right) = \frac{2\pi}{\hbar} \left| \langle i \mid V \mid f \rangle \right|^2 \delta \left(E_i - E_f \right), \tag{4}$$

where $\delta f_{\mathbf{n}}$ is the deviation of the distribution function from Fermi-Dirac equilibrium ($\delta f_{\mathbf{n}}(k) \equiv f_{\mathbf{n}}(\mathbf{k}) - f_{\mathbf{n}}^{\mathrm{FD}}(\mathbf{k})$) for the (sub)band labeled by $\mathbf{n}$, $E_{\mathbf{n}}(\mathbf{k})$ and $\tau_{\mathbf{n}}(\mathbf{k})$ are respectively the energy and relaxation time for a state with wavevector $\mathbf{k}$ (and k the component along the direction of the electric field) in (sub)band $\mathbf{n}$, q is the electron charge, $\mathbf{E}$ the electric field, E_{F} the Fermi energy, V the scattering potential and $\mathbf{J}$ the current density. The dimensionality of $\mathbf{n}$ and $\mathbf{k}$ depends on the system under consideration. The wavevectors $\mathbf{k}$ are one-dimensional ($D = 1$) for nanowires and two-dimensional ($D = 2$) for thin films, while $\mathbf{n}$ is a two-dimensional subband index vector for two-dimensional nanowire confinement and one-dimensional for thin film confinement (including an extra band index in both cases if required). The list of equations follows from the solution of the linearized Boltzmann equation at zero temperature [8]. The linearization and zero temperature assumption are justified in the case of small electric fields, elastic scattering and low enough temperatures ($k_{\mathrm{B}}T \ll E_{\mathrm{F}}$, with E_{F} measured from the lowest conduction band) and these are very reasonable assumptions for typical metallic nanowires and thin films at room temperature with electrons predominantly subjected to grain boundary and surface roughness scattering. All the states $|\mathbf{n}^{(')}\mathbf{k}^{(')}\rangle$ that are considered in Eqs. (1)–(4) are therefore Fermi level states with $E_{\mathbf{n}}(k) = E_{\mathbf{n}'}(k') = E_{\mathrm{F}}$.

The relaxation times in Eq. (2) are coupled self-consistently through a system of linear equations and can be obtained through a matrix (of finite size for a nanowire while requiring numerical discretization of $\mathbf{k}$ for thin films) inversion. Fermi's golden rule is invoked to obtain the scattering rates between the different electron states due to grain boundary and boundary surface roughness scattering. These scattering rates are averaged over an ensemble of grain boundaries and surface roughness profiles to retrieve a general and analytical expression which can be inserted into Eq. (3), allowing for fast and accurate simulations. Because electron-phonon and imperfection (e.g. point defects or impurities) scattering in thin films and nanowires do not deviate much from their bulk scattering behavior while being isotropic and independent from grain boundary and surface roughness scattering (Matthiessen's rule), their resistivity contribution is very close to the bulk value, ρ^{bulk}, and can be separated from the scaling part due to grain boundaries and surface roughness, ρ^{scaling}. This consideration leads to a total resistivity $\rho^{\mathrm{bulk}} + \rho^{\mathrm{scaling}}$, with ρ^{bulk} the bulk resistivity extracted from experiments and ρ^{scaling} resulting from the solution of Eqs. (1)–(4).

The input which is required to solve Eqs. (1)–(4) consists of a correct band structure profile of the nanowire or thin film, to be used in Eqs. (1)–(3), the wave functions of the electron states close to the Fermi level and expressions for the grain boundary and surface roughness potentials, entering the matrix elements in Eq. (4). The set of equations has no remaining free fitting parameters and the resistivity can be obtained without numerical integration.

For grain boundaries, we have borrowed the scattering potential and its distribution from the Mayadas-Shatzkes model [2]:

$$V^{\mathrm{GB}}(x,y,z) = \sum_{\alpha=1}^{N} S^{\mathrm{GB}} \, \delta \left(z - z_\alpha \right), \tag{5}$$

$$g\left(z_1, \ldots, z_N\right) = \frac{\exp\left[-\sum_{\alpha} \left(z_{\alpha+1} - z_\alpha - D^{\mathrm{GB}} \right)^2 / 2 \left(\sigma^{\mathrm{GB}} \right)^2 \right]}{L_z \left[2\pi \left(\sigma^{\mathrm{GB}} \right)^2 \right]^{(N-1)/2}}, \tag{6}$$

where the grain boundaries are represented by N Dirac delta barrier planes normal to the transport (z) direction at positions z_α, the barrier strength S^{GB} being distributed along the wire with an average distance D^{GB} in between subsequent grain boundaries and standard deviation σ^{GB}. The average distance and standard deviation can be estimated from the experimental grain distribution while the barrier strength (having units of energy times length), representing the height and width of the grain boundary potential barrier, can be extracted from ab initio simulations. It typically depends on the orientation of the grains and their boundaries, but gives values of the order of magnitude of eV·Å. The normal orientation of the grain boundary planes in the Mayadas-Shatzkes model can be extended to random orientations but the deviations in resistivity from the results of grain boundaries with normal orientation are quite small [9].

For surface roughness, we consider the following potential and statistics, based on Ando's surface roughness scattering model [10]:

$$V^{\mathrm{SR}}(\mathbf{r}) = U\left(x - \Delta(\mathbf{R}), y, z \right) - U\left(\mathbf{r} \right), \tag{7}$$

$$\langle \Delta\left(\mathbf{R} \right) \rangle = 0, \quad \langle \Delta(\mathbf{R}) \Delta(\mathbf{R}') \rangle = \Delta^2 e^{-(\mathbf{R}-\mathbf{R}')^2 / (\Lambda^2/2)}, \tag{8}$$

where $\mathbf{r} \equiv (x,y,z)$ and we assume a roughness function $\Delta(\mathbf{R})$ with $\mathbf{R} \equiv (y,z)$ that shifts the potential $U(\mathbf{r})$ along a confinement (x) direction as a function of the boundary position $\mathbf{R}$ with zero average, standard deviation (or RMS) Δ and correlation length Λ. The matrix element is linear in V but not linear in Δ. One often expands the matrix element linearly in the roughness function in combination with considering an infinite potential well for $U(\mathbf{r})$, leading to the so called Prange-Nee approximation for surface roughness scattering [11]. This approximation neglects the oscillatory behavior of the wave functions and can lead to large errors on the scattering rates. We have recently introduced an analytical expression for the matrix elements going beyond the linear expansion restriction as well as the infinite potential well limit, hence avoiding additional approximations such as the commonly used Prange-Nee approximation [4]. In this way, the potential barrier outside the wire or film can also be adjusted to represent the surrounding barrier material accurately, improving once again the accuracy of the simulations. While the