Simulation of temperature profile for the electron and the lattice systems in laterally structured layered conductors

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Abstract – Electrons in operating microelectronic semiconductor devices are accelerated by locally varying a strong electric field to acquire effective electron temperatures nonuniformly distributing in nanoscales and largely exceeding the temperature of the host crystal lattice. The thermal dynamics of electrons and the lattice are hence nontrivial and its understanding at nanoscales is decisively important for gaining a higher device performance. Here, we propose and demonstrate that in layered conductors the nonequilibrium nature between the electrons and the lattice can be explicitly pursued by simulating the conducting layer by separating it into two physical sheets representing, respectively, the electron and the lattice subsystems. We take, as an example of simulating GaAs devices, a 35 nm thick, 1 \( \mu \)m wide U-shaped conducting channel with 15 nm radius of curvature at the inner corner of the U-shaped bend, and find a remarkable hot spot to develop due to hot-electron generation at the inner corner. The hot spot in terms of the electron temperature achieves a significantly higher temperature and is of far sharper spatial distribution when compared to the hot spot in terms of the lattice temperature. A similar simulation calculation made on a metal (NiCr) narrow lead of similar geometry shows that a hot spot shows up as well at the inner corner, but its strength and the spatial profiles are largely different from those in semiconductor devices; viz., the amplitude and the profile of the electron system are similar to those of the lattice system, indicating quasi-equilibrium between the two subsystems. The remarkable difference between the semiconductor and the metal is interpreted to be due to the large difference in the electron specific heat, rather than the difference in the electron phonon interaction. This work will provide useful hints to a deeper understanding of the nonequilibrium properties of electrical conductors, through a simple and convenient method for modeling nonequilibrium layered conductors.

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Introduction. – Electro-thermal behavior is a key ingredient for understanding charge carrier transport phenomena in semiconductor devices including two-dimensional (2D) materials, heterojunctions, and strong correlated systems [1–15]. In small devices on nanoscales, hot-electron generation and the resulting characteristic interaction with the host crystal lattice (or phonons) complicates the electro-thermal analysis and limits the device performance [16,17]. Whereas knowing the detailed local profile of the electron effective temperature, \( T_e \), separately from that of the lattice temperature, \( T_L \), in the presence of current is a prerequisite for understanding

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the transport characteristics on nanoscales [18–22], $T_e$ has been experimentally hardly accessible [23–31] until quite recently [32,33]. It follows that the study of electro-thermal properties has so far been restricted only to the simulation methods such as those of the Monte Carlo (MC) simulation based on the Boltzmann transport equations, hydrodynamic equations or molecular dynamics [34–38]. Unfortunately, however, MC simulations comprise involved calculation procedures, which are not necessarily convenient to gain intuitive understanding of the electro-thermal transport phenomena of given devices. On the other hand, the nonequilibrium condition cannot be incorporated in commercially available semiconductor device simulators.

Here, we propose a simplified electro-thermal model for layered conductors on the basis of the assumption that the electron- and the lattice-subsystems are, respectively, in quasi-equilibrium states characterized by the effective electron temperature $T_e$ and the lattice temperature $T_L$. The model is applied to a U-shaped layered conductor, where the electric field is concentrated at the inner corner of the U-shaped bend. In a semiconductor device, simulating GaAs, a remarkable hot-electron distribution ($T_e \gg T_L$) is found to develop at the corner, forming a sharp hot spot with $T_e$ reaching $\sim 2000$ K. Differently, in metal devices, simulating NiCr, hot-electron effects are found to be absent ($T_e \approx T_L$), whereas a hot-spot profile is visible. These findings are consistent with recent experimental results reported on metals [39] and semiconductors [32], indicating the validity of the present model for simulating the electro-thermal behavior of layered conductors in nonequilibrium conditions.

Simulation model. – Figure 1 describes the model conductor considered in this study. A layered conductor with the electric conductivity $\sigma_e$ is deposited on an insulating substrate, which is anchored by the heat sink at 300 K. The lateral shape of the conductor is arbitrary, so that the electric field $E$, the current density $j$, the electron temperature $T_e$ and the lattice temperature $T_L$ in the conductor are variables to be consistently derived as functions of the lateral position $r$ for a given conductor with a given bias voltage. In the conductor electrons gain energy from $E$ through $P = j(r) \cdot E(r) = \sigma_e E^2$ and the energy gained from the field is, in turn, released to the lattice via an electron-phonon interaction, characterized by the electron-phonon energy relaxation time $\tau_{e-ph}$. The excess energy (or heat) of electrons is transferred, as well, within the electron system through the electron thermal conduction $-\kappa_e \nabla T_e$ with $\kappa_e$ the electron thermal conductivity. The heat is transferred similarly within the lattice system through lattice thermal conduction $-\kappa_L \nabla T_L$ with $\kappa_L$ the lattice thermal conductivity. The heat is eventually transferred to the substrate ($T_L - T_{LS})/h_L$ with $h_L$ being the interface thermal resistance and $T_{LS}(r)$ the local lattice temperature of the substrate on its top surface, and finally absorbed by the heat sink. Heat is transferred as well through electrical leads connected to the conductor, as represented by the arrows marked with $\kappa_e$ and $\kappa_L$ in fig. 1(c), which is taken into account in the model through an appropriate boundary condition as mentioned below for fig. 2(a).

As schematically shown in figs. 1(b) and (c), our model represents the energy transfer from the electron system to the lattice system in the conductor by the interface heat transfer between the electron sublayer at $T_e$ to the lattice sublayer at $T_L$. The energy flux released from the electron system to the lattice system through the electron-phonon
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Table 1: Parameters used in the simulation.

| Quantity | $\sigma_e$ | $\kappa_e$ | $\kappa_L$ | $h_{e, ph}$ | $h_I$ | $\kappa_S$ |
|----------|------------|------------|------------|-------------|-------|------------|
| Unit     | S/m        | W/(m·K)    | W/(m·K)    | Km$^2$/W    | Km$^2$/W | W/(m·K)    |
| n-GaAs   | $8.8 \times 10^4$ | 0.1        | 50         | $4.3 \times 10^{-7}$ | 0      | 50         |
| NiCr     | $2.89 \times 10^5$ | 15         | 1          | $2.7 \times 10^{-10}$ | $3 \times 10^{-8}$ | 150       |

interaction is given by

$$P_{e-ph} = (T_e - T_L)C_e/\tau_{e-ph} \tag{1}$$

with $C_e$ the electron specific heat per unit area, so that the effective interface thermal resistance $h_{e-ph}$ is

$$h_{e-ph} = \tau_{e-ph}/C_e. \tag{2}$$

The specific heat is approximated by

$$C_e = C_{ec} = (3/2)N_{2D}k_B, \tag{3}$$

for a classical electron system ($k_B T_e \gg \varepsilon_F$) and by

$$C_e = C_{eF} = (3/2)k_B T_e/\varepsilon_F C_{ec} \tag{4}$$

for an electron system with the Fermi energy $\varepsilon_F$ much higher than the thermal energy ($k_B T_e \ll \varepsilon_F$). Here, $k_B$ is the Boltzmann constant, and $N_{2D}$ is the 2D electron density.

**Simulated structure.** – As schematically illustrated in fig. 2(a), we consider a 35 nm thick conductor layer shaped into a 1 μm wide U-shaped channel where the radius of the inner curvature of the U-shape is 15 nm and the gap between the channels is $S = 30$ nm. For the simulation, the electron and the lattice systems of the conducting channel are separately represented by Layers A and B, where Layer B is placed on the 10 μm thick substrate (Layer C). The boundary condition of temperature is given by assuming $T = 300$ K on the bottom face Layer C and on the end faces of Layers A and B as marked by the orange lines in fig. 2(a). As to the bias condition, a constant voltage is assumed on each end face of the conducting channel (Layer A), and a bias voltage $V_b$ is assumed to give the voltage difference between the two end faces.

Two different conductors are considered. One is a doped n-GaAs channel and the other is a NiCr channel, similar to those studied, respectively, in refs. [32] and [39]. Substrates are assumed to be lattice-matched GaAs/AlGaAs for the n-GaAs sample [32] and single crystal Si covered with a thin SiO$_2$ layer for the NiCr sample [39]. The electron density in n-GaAs and NiCr samples is, respectively, $N_{2D} = 3.3 \times 10^{24}$/m$^2$ and $1.0 \times 10^{20}$/m$^2$; in terms of the sheet electron density, $N_{2D} = 1.1 \times 10^{17}$/m$^2$ and $3.5 \times 10^{22}$/m$^2$. The specific heat is taken to be $C_e = 2.3 \times 10^{-6}$Ws/(Km$^2$) and $1.1 \times 10^{-2}$Ws/(Km$^2$), respectively assuming eqs. (3) and (4) for n-GaAs and NiCr samples. In the n-GaAs sample, the interface thermal resistance ($h_I$) is negligibly small because the n-GaAs conducting layer is epitaxially grown on the lattice-matched substrate. The electron-phonon energy relaxation time is assumed to be $\tau_{e-ph} = 1$ ps and 3 ps, respectively for n-GaAs [32] and NiCr [39]. The parameter values used are summarized in table 1.

**Results and discussions.** – With the finite-element method in a commercial multiphysics software (COMSOL), the heat arising from electrically biased conductors can be simulated according to Ohm’s law and Joule’s law in the electromagnetics module and then dissipated through Fourier’s law of heat conduction in the lattice systems is largely different as described in detail below. It is a common feature of both n-GaAs and NiCr samples that the electric field is concentrated around the U-shaped inner corner as exemplified by the result for the n-GaAs sample: The electric field is nearly uniform and $E = 2$–$3$ kV/cm in a region away from the U-shaped corner, but it rapidly increases to reach about $E = 10$ kV/cm in the vicinity of the U-shaped corner.

As a consequence of this $E$-field enhancement, remarkable nonuniform hot-electron distribution is found to be generated at the inner corner of the n-GaAs sample as shown in fig. 2(c). While the trend of the $E$-field enhancement is substantially the same in the NiCr sample, the resulting temperature distribution in the electron and the lattice systems is largely different as described in detail below.

Figures 3(a), (b) and figs. 4(a)–(d) display the distributions of $T_e$ (Layer A) and $T_L$ (Layers B) for the NiCr sample. The profile of $T_e$ is similar to that of $T_L$, and both exhibit spatially varying heating in accord with the $E$-field enhancement peaked at the U-shaped inner corner. The highest temperature at the hot spot is about 150°C above the heat sink (300 K). The amplitude of the temperature rise at the hot spot ($\Delta T_e \approx 150$°C) as well as the quasi-equilibrium feature between the electron and the lattice systems ($T_e \approx T_L$) substantially reproduce the experimental findings reported in ref. [39].

The feature of the hot-spot formation is largely different in the n-GaAs sample as shown in figs. 3(c), (d) and
The electron temperature $T_e$ is much higher than the lattice temperature $T_L$, indicating nonequilibrium hot-electron generation, and it assumes a very sharp prominent peak reaching as high a value as $T_e \sim 2000$ K. On the other hand, the highest value of $T_L$ ($<330$ K) is at most only $\sim 30$ °C above the temperature of the heat sink (300 K). In addition, the hot-spot feature is practically missing as evident in figs. 4(f) and (h). The generation of remarkable hot-electron distribution is consistent with the experimental finding reported on n-GaAs constriction devices [32].

The large difference in the electro-thermal properties noted between the n-GaAs sample and the NiCr sample in this study is suggested to be generally inherent to semiconductors and metals. When the energy flux $P$ is fed to the electron system in a steady state, the electrons are heated above the lattice temperature by

$$T_e - T_L = (\tau_{e-ph}/C_e)P = h_{e-ph}P$$

if the temperature gradient is ignored. For a given $P$, the rise of $T_e$ is proportional to $\tau_{e-ph}$ and $1/C_e$. In general, $\tau_{e-ph}$ is not largely different between semiconductors and metals, but the heat capacity $C_e$ is by orders of magnitude smaller in semiconductors because the electron density is far lower. It follows that the electron system is readily driven away from the equilibrium with the lattice in semiconductors. In terms of our model ($h_{e-ph}$), the thermal contact between the electron and the lattice systems is weak in semiconductors so that they are readily driven out of equilibrium. We mention that a high mobility of electrons is often ascribed to be the cause of hot-electron generation in semiconductors. The present study makes this assumption questionable; namely, a high mobility implies a high electrical conductivity (and a large $P$), but the electrical conductivity is usually higher in metals and does not explain why a semiconductor is more feasible for hot-electron generation.

In this study the simulation calculation assumed linear transport. Namely the electrical conductivity and the thermal conductivities are assumed to be constants. In metals, nonlinear effects may not be significant since the $T_e$ rise is not too large. In the doped n-GaAs sample at room temperature (as in this work), nonlinear effects may not be serious up to $E \approx 10$ kV [32], so that the findings in the present study are supposed to be valid. In the higher-$E$ region above 10 kV/cm, however, the electron mobility will be reduced due to the transfer of electrons to upper (X and/or L) valleys. Even in such a higher-$E$ region, our model will provide a useful guideline at the starting point.

**Summary.** We demonstrate that in layered conductors the nonequilibrium nature between the electrons and the lattice can be explicitly pursued by separating the electron and the lattice subsystems into two physical layers that exchange heat at the interface. Highly nonequilibrium distribution of electrons from that of the lattice is found in a doped n-GaAs sample. In a NiCr sample with a similar configuration, the electron and the lattice systems are in quasi-equilibrium. Remarkable difference of the electro-thermal properties of semiconductors and metals is suggested to arise from the difference in the electron specific heat. This work provides a simple and convenient method for modeling layered conductors in a nonequilibrium condition, and will give useful hints for deeper understanding of the nonequilibrium properties of electrical conductors.
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