A computational model for the investigation of phonon-limited charge transport in 2D systems

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A computational model has been developed for phonon-limited charge transport in 2D systems. Currently, this model is used to study transport in graphene and silicon thin films. The results obtained so far show a good agreement with experiments.

The model is based on an atomistic approach considering full electronic band structure and all phonon branches. The electronic band structure is calculated with a tight-binding model (Fig. 1). The phonon dispersion is computed with the Vanderbilt force field model [1] for silicon thin films, and with a force constant method [2] for graphene using parameters fitted to the density function theory (Fig. 2). All possible electron-phonon scattering processes are searched in the energy window relevant for transport by checking if any phonon satisfies energy and momentum conservation rules. The rate of each scattering process is calculated by Fermi golden rule. These scattering rates are then used in Boltzmann transport equation to compute the response of the electron distribution to a low electric field, then the resistivity and the mobility are determined.

The tight-binding parameters of graphene and their dependence on strain have been extracted from *ab-initio* calculations. Generally, for graphene on a oxidized substrate, the resistivity consists of three major components:

$$\rho(T) = \rho_0 + \rho_{ph}(T) + \rho_{SO}(T), \qquad (1)$$

where T is temperature, ρ_0 is due to impurities, ρ_{ph} is due to the intrinsic phonons of graphene, and ρ_{SO} is due to the surface optical phonons of the substrate [3]. Here, graphene on SiO_2 was considered. Fig. 3 compares the results of the simulation (represented by a green dotted line) with the experimental data [4] (represented by red markers) in a wide range of temperature and at three different electron densities. It is clear that they agree very well with each other. Fig. 4 shows the temperature dependence of ρ_{ph} and ρ_{SO}. It can be concluded that the intrinsic phonon scattering dominates the temperature dependent resistivity of graphene at sufficiently high carrier concentration. Fig. 5 shows the carrier density dependence of ρ_{ph} and ρ_{SO} at 300K. ρ_{ph} is asymmetric respect to the charge neutrality point, because the carrier-phonon coupling is not the same for hole states and electron states.

In silicon thin films, it is known that the conduction band acoustic deformation potential D_{ac} has to be increased from $D_{ac} \sim 10$ eV in bulk to $D_{ac} \sim 15$ eV in thin films to match the experimental electron mobility [5]. We are therefore exploring this problem from a tight-binding perspective to get a better insight into the underlying physics. So far, we have investigated the mobility in $[001]$ silicon thin film (thickness < 5 nm) at low carrier density (Fig. 6). More comprehensive data on thicker films and as a function of carrier density/effective electric field will be discussed at the conference.

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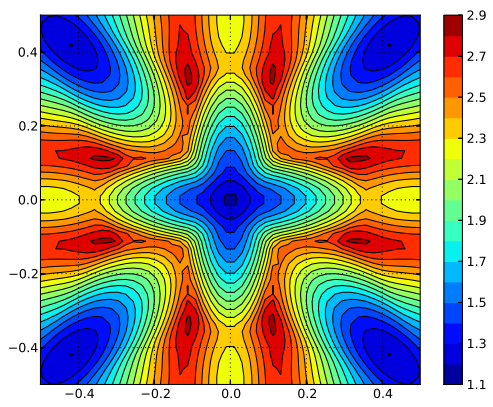

Fig. 1. Electronic band structure of a 4 nm thick silicon film calculated with tight-biding method.

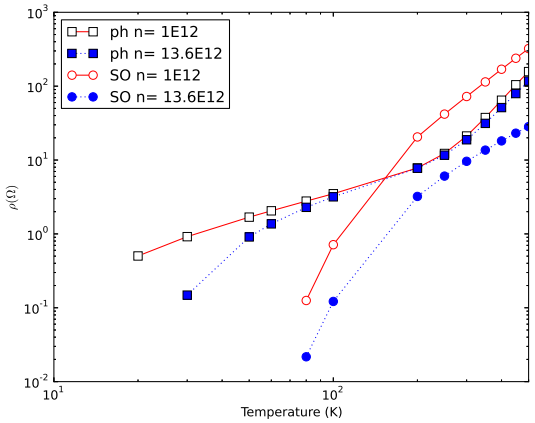

Fig. 4. ρ_{ph} (square makers) and ρ_{SO} (circle markers) versus temperature at electron densities 1 and 13.6×10^{12} cm ^{2}.

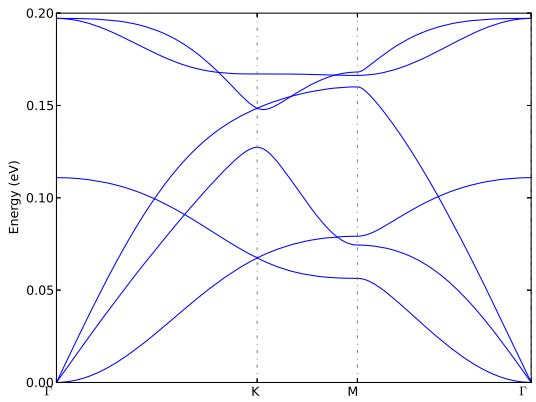

Fig. 2. Phonon dispersion of Graphene calculated by a force constant method [2] using parameters fitted to the DFT.

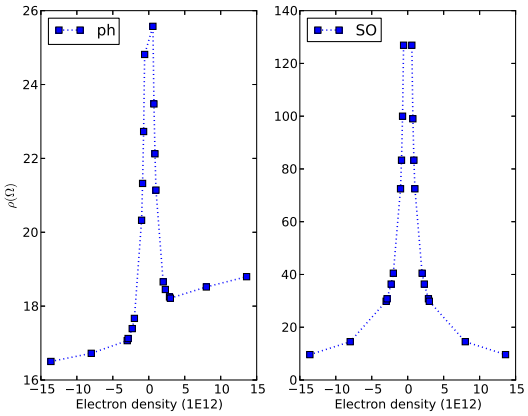

Fig. 5. ρ_{ph} (left) and ρ_{SO} (right) versus charge density at 300K.

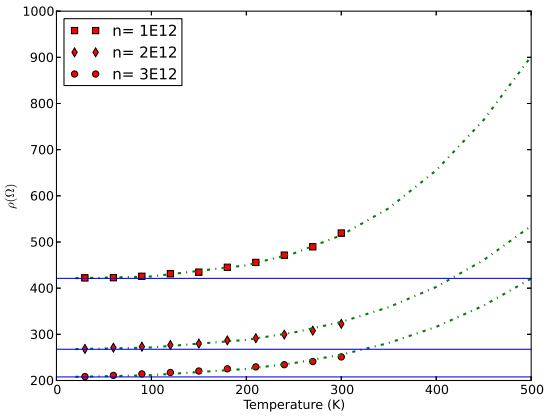

Fig. 3. Comparison of simulations (dotted lines by setting ρ_0 at the solid lines) and experimental data (red markers) [4].

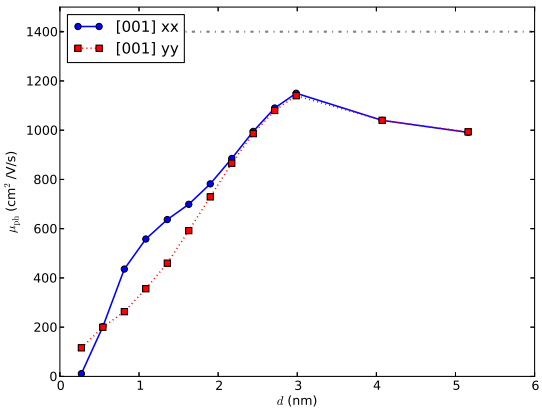

Fig. 6. Low field mobility of $[001]$ silicon thin film in $[1\bar{1}0]$ (xx) and $[110]$ (yy) directions. The gray dotted line is the mobility of bulk silicon.