Effects of charged impurity clusters on the conductivity of supported graphene

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Charged impurities are likely to be introduced into graphene samples by typical fabrication and processing techniques, and can persist even after annealing [1]. Such impurities are likely to produce electron-hole puddles with an average size of 20 nm [2]. These electron-hole puddles point towards a clustered impurity distribution, as opposed to a uniform random distribution. It has also been shown that spatially correlated impurities affect the conductivity of graphene [3, 4]. Therefore, a reliable and quantitative determination of the effects of such impurities on carrier transport in graphene supported on SiO_2 is important for the development of graphene-based applications. We have combined particle-based transport simulations, using the ensemble Monte Carlo (EMC) method, with numerical long-range and short-range field solvers, using the finite-difference time-domain (FDTD) technique and molecular dynamics (MD), respectively, in order to simulate the formation of electron-hole puddles and study the effect of charged impurity distributions on the conductivity of graphene supported on SiO_2. The coupled EMC-FDTD-MD algorithm has been used to calculate the high-frequency conductivity of bulk silicon [5, 6] in very good agreement with experimental data.

We simulate a structure consisting of a monolayer of graphene on top of an SiO_2 substrate. Clusters of impurity ions are present at and near the interface between graphene and the substrate. The charged impurity clusters are stochastically initialized using a correlation length parameter to define the average size and distribution of the clusters. By simulating carrier dynamics without any external fields, we have calculated the steady-state electron and hole density distributions for a uniform random, as well as a clustered impurity distribution. The average size of the electron-hole puddles, which is calculated using the full width at half maximum of the normalized spatial auto-correlation functions of the density distributions, are about 4 nm and 20 nm for the uniform random and clustered impurity distributions, respectively. We show that impurity clusters between the sizes of 30 and 40 nm are responsible for producing electron-hole puddles quantitatively similar to those seen in experiments [2]. We also calculated the conductivity in graphene as a function of the carrier density, for impurity-free, as well as for uniform random and clustered impurity distributions, with an impurity density of 10^{11}–10^{12} cm^{-2} and an average cluster size of 36 nm. We show that, for impurity densities greater than 10^{11} cm^{-2}, the distribution of impurities (random or clustered) significantly affects both the sublinearity and the slope of the linear region in the carrier-density dependence of conductivity. By turning off/on specific terms in the MD to elucidate the effect of short-range carrier-carrier and carrier-ion interactions, we find that the sublinearity in conductivity as a function of the carrier-density is due to direct and exchange carrier-carrier interactions limiting transport. Moreover, the slope of the linear region is strongly dependent on the short-range carrier-ion Coulomb interaction, and therefore on the density and distribution of the impurities.

In conclusion, we quantitatively show that clustered impurities, as well as the resulting short-range carrier-ion, and carrier-carrier interactions, play an important role in determining the room-temperature conductivity of supported graphene.

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