MAR13-2012-020092

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Pseudopotential-based study of electron transport in low-dimensionality nanostructures

MASSIMO FISCHETTI, Department of Materials Science and Engineering, University of Texas at Dallas

Pseudopotentials– empirical and *ab initio* – are now being more commonly used to study not only the atomic and electronic structure of nanometer-scale systems, but also their electronic transport properties. Here we shall give a bird-eye view of the use of density functional theory (DFT) to calibrate empirical pseudopotentials (EPs), of EPs to calculate efficiently the electronic structure of low-dimensionality systems, the most significant electronic scattering processes, and to study semiclassical and quantum electronic transport. Low-dimensionality systems considered here include thin semiconductor layers, graphene, graphene- and silicane-nanoribbons, and silicon nanowires. Regarding graphene, the high electron mobility measured in suspended graphene sheets ($\sim$ 200,000 cm^2/Vs) is the result of a relatively weak carrier-phonon and the strong dielectric-screening property. However, in practical applications graphene is likely to be supported by an insulating substrate, top-gated, and possibly used in the form of narrow armchair-edge nanoribbons (aGNRs) in order to open a gap. We will discuss several scattering processes which may affect the electron transport properties in these situations. First, we shall present results of the calculation of the intrinsic electron-phonon scattering rates in suspended graphene using empirical pseudopotentials and the rigid-ion approximation, resulting in an electron mobility consistent with the experimental results. We shall then discuss the role of interfacial coupled substrate optical-phonon/graphene-plasmons in depressing the electron mobility in graphene supported by several insulators (SiO_2, HfO_2, Al_2O_3, and h-BN). We shall also discuss the role of Coulomb scattering with charged defects/impurities in gated graphene sheets and the role of the metal gate in screening this interaction. Finally, we shall review the strong effect of line edge roughness (LER) on electron transport and localization in narrow aGNRs resulting from the "aromatic" width dependence of the band-gap of the sp^2-coordinated aGNRs. This will lead us to consider sp^3-coordinate ribbons (silicane) and Si nanowires as possible alternative structures – less affected by LER scattering – of interest in nanoelectronics application.