

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

M. V. Fischetti¹, S. J. Aboud², Z.-Y. Ong¹, J. Kim¹, S. Narayanan¹, and C. Sachs¹¹Department of Materials Science and Engineering, University of Texas at Dallas,

800 W. Campbell Rd., Richardson, TX 75080

²Energy Resources Engineering Department, Stanford University, 367 Panama Street, Stanford, CA 94305

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's-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 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 sheets¹ (~200,000 cm²/Vs, as seen in the theoretical results shown in Fig. 2) is the result of a relatively weak carrier-phonon coupling 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 electron transport in these situations. First, we shall present results of the calculation of the intrinsic electron-phonon scattering rates in suspended graphene and AGNRs using empirical pseudopotentials² and the rigid-ion approximation³ or DFT calculated deformation potentials⁴ (see Fig. 1), resulting in an electron mobility consistent with the experimental results (as shown in Figs. 2 and 3). We shall then discuss the role of interfacial coupled substrate optical-phonon/graphene-plasmons⁵ (*i.e.*, remote phonons) in depressing the electron mobility in graphene supported by SiO₂, HfO₂, Al₂O₃, and h-BN, as shown in Fig. 4. Finally, we shall review the strong effect of line edge roughness (LER) on electron transport (Fig. 5) and localization in narrow AGNRs⁶ resulting from the 'aromatic' width dependence of the band-gap of the *sp*²-coordinated ribbons (silicane) and Si nanowires as possible alternative structures -- less affected by LER scattering -- of interest in nano-electronics application.

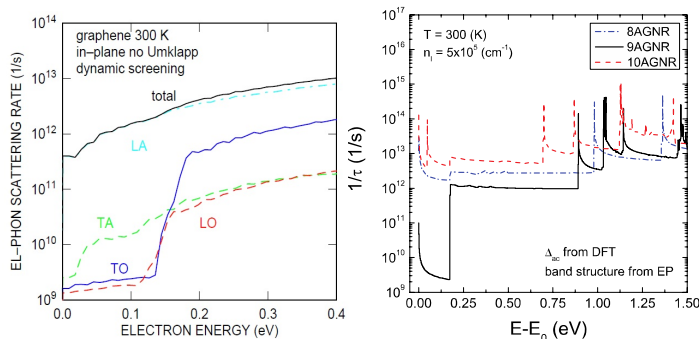


Fig. 1 *Left*: Electron-phonon scattering rates in suspended graphene at 300K calculated using EPs and the rigid-ion approximation. *Right*: Electron momentum relaxation rate in AGNRs of various width calculated using DFT-determined deformation potentials, as in Ref. 4.

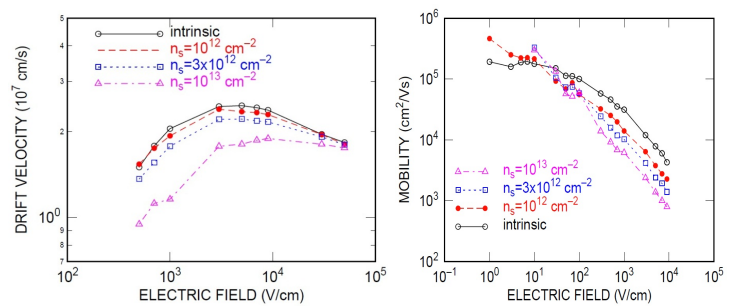


Fig. 2 Electron drift velocity vs. field (left) and longitudinal mobility vs. field calculated from the rates shown in Fig. 1 (left) at various values of the electron density.

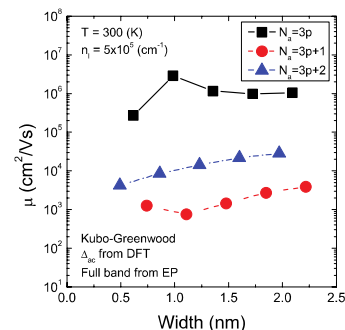


Fig. 3 Electron mobility in AGNRs of various widths calculated using the momentum relaxation rates shown in Fig. 1 (right).

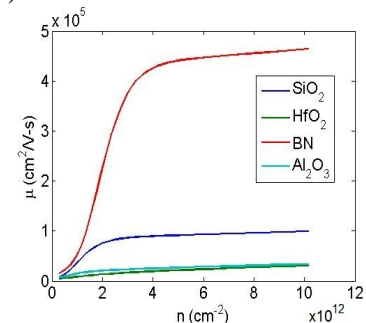


Fig. 4 Calculated remote-phonon-limited electron mobility in graphene supported by the insulators shown.

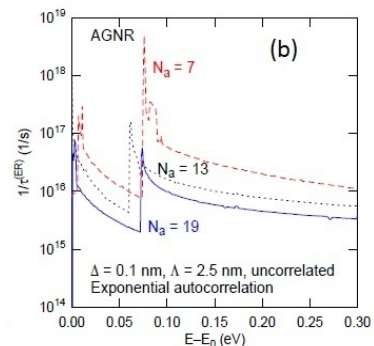


Fig. 5 Electron-LER scattering rates in AGNRs. Note the magnitude of the rates which show the breakdown of perturbation theory and suggest electron localization..

References

1. K. Bolotin *et al.*, Solid State Comm. **146**, 351 (2008).
2. Y. Kurokawa, S. Nomura, T. Takemori, and Y. Aoyagi, Phys. Rev. B **61**, 12616 (2000).
3. S.J. Aboud, M. Saraniti, S.M. Goodnick, and M. V. Fischetti, in "Proc. International Workshop on Computational Electronics", pp. 93-94 (2012).
4. M. O. Long, L. Tang, D. Wang, L. Wang, and Z. Shuai, J. Am. Chem. Soc. **131**, 17728 (2009).
5. Z.-Y. Ong and M. V. Fischetti, Phys. Rev. B **86**, 165422 (2012); *ibid.* **86**, 199904(E) (2012).
6. M. V. Fischetti and S. Narayanan, J. Appl. Phys. **110**, 083713 (2011).