Full band Monte Carlo simulation of electron transport in thin Si and Graphene

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***Abstract*— Electron transport in nanostructures is studied using self-consistent Monte Carlo/Poisson simulations based on empirical pseudopotentials to calculate the band structure – using the supercell method – and to obtain the electron-phonon scattering rates using the rigid-ion approximation. The two cases of thin Si bodies and graphene are considered and we compare our results with those obtained employing the commonly employed empirical deformation potentials for the electron-phonon matrix elements. We emphasize the difference between the low-field mobility and saturated velocity in Si and C-based structures.**

INTRODUCTION

The excellent electrical and thermal properties of graphene has attracted tremendous research interest for potential device applications.[1]. It is interesting to study and compare the performance of Si and graphene at dimensions below $10-15$ nm, where carbon based devices could potentially replace Si. The study of electronic transport in nanoscale devices like thin Si thin bodies and graphene requires an accurate description of their band structure, which is provided by the use of empirical pseudopotentials[2] coupled with the supercell method. Furthermore, we discuss semiclassical transport through Monte-Carlo simulations[3] after evaluation of electron-phonon scattering rates. The electron-phonon interactions are treated employing both deformation potential approach and rigid-ion approach.

SIMULATION MODEL

To determine the band structure, we solve the Schrödinger equation given by:

$$\sum_{\mathbf{G}'}\left[\frac{\hbar^2}{2m}|\mathbf{k}+\mathbf{G}|^2\delta_{\mathbf{G},\mathbf{G}'}+V^{(lat)}_{\mathbf{G},\mathbf{G}'}+V^{(ext)}_{\mathbf{G},\mathbf{G}'}\right]\mathbf{u}^{(n)}_{\mathbf{G}',\mathbf{k}}= E_n(\mathbf{k})\mathbf{u}^{(n)}_{\mathbf{G}',\mathbf{k}}, \quad (1)$$

where $V^{(lat)}_{\mathbf{G},\mathbf{G}'}$ is the fourier component of the lattice potential which contains the empirical pseudopotential parameter. The Schrödinger equation is solved iteratively with the Poisson equation to obtain the band structure for a self-consistent field. The electron-phonon scattering rate is given by:

$$\frac{1}{\tau^{(\eta)}_n(\mathbf{K})}=\frac{2\pi}{\hbar}\sum_{\mathbf{K}',n',\mathbf{q}}|\langle\mathbf{K},n|V^{(\eta)}_{\mathbf{q}}|\mathbf{K}',n'\rangle|^2\times \delta[E_n(\mathbf{K})-E_{n'}(\mathbf{K}')\pm\hbar\omega^{(\eta)}_{\mathbf{q}}], \quad (2)$$

where, the scattering potential $V^{(\eta)}_{\mathbf{q}}$ is parameterized empirically in deformation potential approaches, whereas it is calculated using the rigid-ion approximation in our empirical-pseudpotential-based approach. With the electron-phonon scattering rates, velocity-field characteristics are generated using a Monte-Carlo technique.

RESULTS AND CONCLUSIONS

For a thin inversion layer, the band structure was evaluated for a self-consistent field with a sheet density of $10^{13}cm^{-2}$ as shown in Fig. 1. The scattering rates for this structure were evaluated using both deformation potential method as shown in Fig. 2 and using the more rigorous rigid-ion method as shown in Fig. 3 and there is a good agreement between them. In Fig. 4, the velocity-field characteristics for the same structure obtained using a Monte-carlo technique is shown. The scattering rates from Fig. 2 were used for this purpose. The Figure 5 shows the electron-phonon scattering rates of graphene using a rigid-ion approach. Similar calculations performed for single-layer graphene will also be presented and a comparison will be drawn to assess the relative merit of Si- and C-based devices.

REFERENCES

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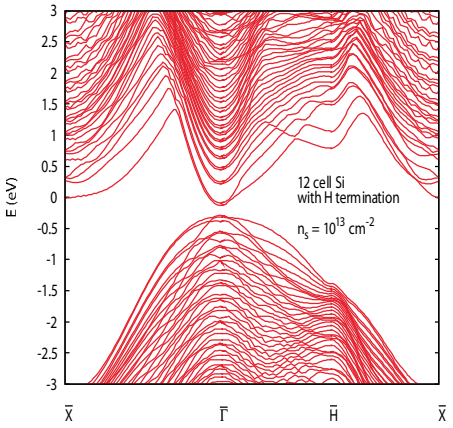

Fig. 1. Band structure of 12 cell Si with H termination under a self-consistent field with a sheet density of $10^{13}\ cm^{-2}$.

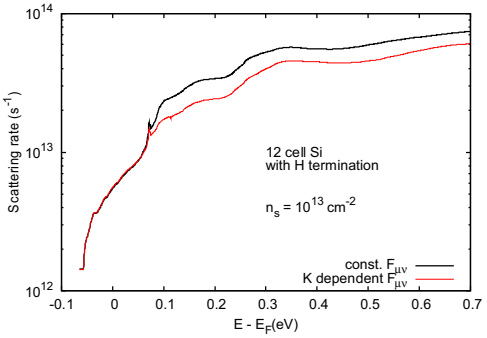

Fig. 2. Electron-Phonon scattering rates in 12 cell Si with H termination evaluated using deformation potentials

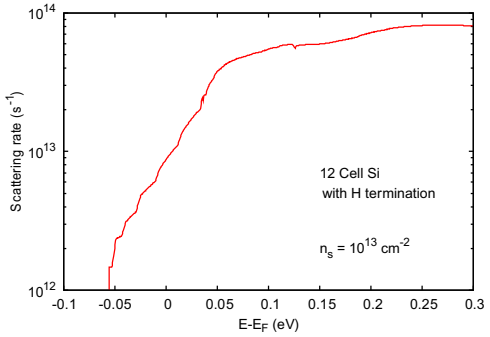

Fig. 3. Electron-Phonon scattering rates in 12 cell Si with H termination evaluated using rigid ion model.

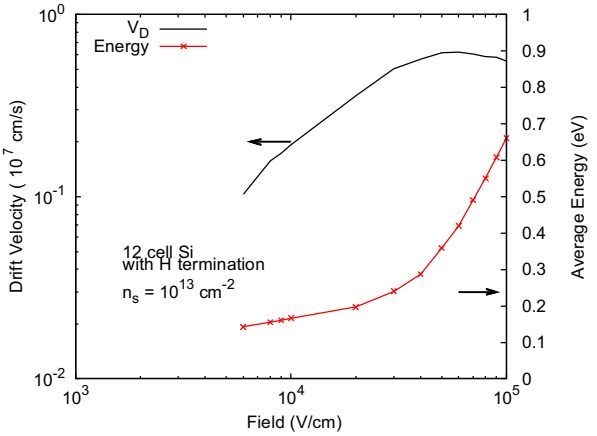

Fig. 4. Velocity-Field Characteristics in 12 cell Si with H termination using Monte-Carlo simulations.

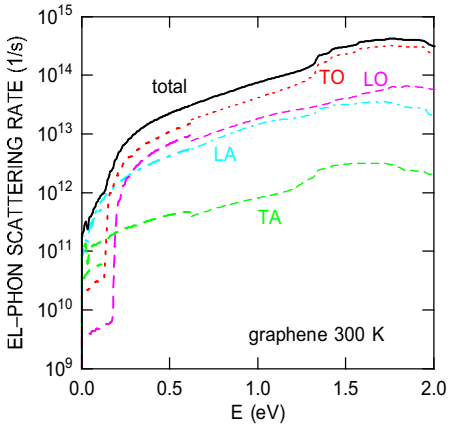

Fig. 5. Electron-Phonon scattering rates in graphene using rigid ion model