Calculation of Electron-Phonon Interaction Strength from First Principles in Graphene and Silicon

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INTRODUCTION

The calculation of electron-phonon interaction from first principles has recently become feasible using density-functional perturbation theory (Quantum Espresso) [1] and the small displacement method (GPAW) [2]. We determine the strength of the electron-phonon interaction using the Vienna Ab-Initio Simulation Program (VASP) [3] with the small displacement method using PHONOPY [4]. We illustrate our approach using graphene and calculate the interband deformation potentials for bulk Si relevant for Band-to-Band Tunneling (BTBT).

ELECTRON-PHONON INTERACTION

We first use VASP to calculate the electronic bandstructure of the materials under study with the ions in their equilibrium position as shown in Fig. 1 for graphene. The phonons are calculated by constructing a supercell and calculating the force constants using small displacements using PHONOPY. The resulting phononic band structure for graphene is shown in Fig. 2.

To determine the strength of the electron-phonon interaction, we displace each atom in three orthogonal directions and the three opposing directions. We extract the Hartree part of the Kohn-Sham potential (shown in Fig. 3) for each displacement which allows us to determine

\[
\frac{\partial V_H(r)}{\partial \mathbf{R}_i} \approx \frac{V_H(r)|_{+\delta} - V_H(r)|_{-\delta}}{2|\delta|}
\]

using central difference as illustrated in Fig. 4.

We Fourier transform the wavefunctions to real-space and calculate the deformation potential as

\[
DK'_{k,q} = \sum_{r,i} \psi^*_{k+q,r}(r)\psi_{k,r}(r)M_i\mathbf{e}_{q,i}\cdot \frac{\partial V_H(r)}{\partial \mathbf{R}_i}
\]

where \( \nu \) is the phonon branch index and \( \mathbf{e}_{q,i} \) are the normalized displacement vectors, \( M_i \) are the ion masses and \( M \) is the unit cell mass.

GRAPHENE AND SILICON

Fig. 5 shows the electron-phonon matrix elements for graphene. The difference in symmetry between the lowest conduction band at \( \Gamma \) and the conduction band near \( K \) result in a discontinuity in the electron-phonon strength half-way along the \( \Gamma - M \) and \( \Gamma - K \) lines where a band crossing occurs. From Fig. 5 it can be seen that near \( K \), transitions to the \( K \)-point due to ZA and ZO phonons are prohibited while near \( \Gamma \), transitions to the \( K \)-point due to LA, TA, LO and TO phonons are prohibited.

In Fig. 6, we show the electron-phonon interaction in silicon for electrons starting at the valence band at \( \Gamma \) going towards the conduction band. The deformation potentials relevant for BTBT can be found 0.85 along the \( \Gamma - X \) axis and measures \( 3.5 \times 10^8 \) eV/cm, \( 8.7 \times 10^8 \) eV/cm and \( 3.3 \times 10^8 \) eV/cm for TA, LO and TO phonons respectively. This suggests that a previous estimate [5] of \( 2.45 \times 10^8 \) eV/cm for the interaction with the TA and \( 5.6 \times 10^8 \) eV/cm for the interaction with the TO was an understimation while the interaction with LO which is usually not considered is of similar strength as the TO.

CONCLUSION

Determining the electron-phonon interaction strength from first principles can give a quick overview of which electron-phonon interactions will dominate. We have shown that for BTBT in silicon, the LO phonon interaction which is usually ignored is important while interaction with TA and TO may have been underestimated.

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REFERENCES

Fig. 1. Electronic band structure of graphene as calculated by VASP.

Fig. 2. Phononic band structure for graphene as calculated by VASP.

Fig. 3. Hartree part of the Kohn-Sham potential calculated for graphene as calculated by VASP averaged along the $z$-direction.

Fig. 4. The change in the Hartree part of the Kohn-Sham potential for graphene with a small displacement of the center atom in the $x$ direction averaged along the $z$ direction.

Fig. 5. Graphene electron-phonon deformation potentials for electrons starting at the K-point going to the lowest conduction band.

Fig. 6. Silicon electron-phonon interaction strength starting from the $\Gamma$-point valence band to the first conduction band.