Influence of Deformation Potential Scattering on Impact Ionization in Ultra-Wide Bandgap Materials

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INTRODUCTION

A major advantage of ultra-wide band gap (UWBG) materials for power electronic applications are the predicted high breakdown voltages limited by avalanche breakdown due to impact ionization. However, experimental data on the impact ionization coefficients in these new class of materials is limited. Theoretical calculations of ionization coefficients using Monte Carlo methods are highly influenced by the choice of impact ionization and deformation potential scattering rates, which in turn are dependent on the electronic structures and phonon dispersions used as inputs. In the present paper, we present comparisons of the impact ionization and electron-phonon deformation potential scattering rates using various combinations of pseudopotential, electronic structure, and phonon dispersion inputs.

MODEL

The impact ionization and electron-phonon deformation potential scattering rates are computed from Fermi's golden rule. Electronic structures are computed from DFT using Quantum Espresso and from GW using BerkeleyGW. Phonon dispersions are calculated from DFPT using Quantum Espresso and from an empirically fitted valence force field model. K-vector dependent deformation potentials are computed using EPW in Quantum Espresso. The impact ionization coefficient is calculated from full band cellular Monte Carlo (CMC) simulation as shown in Fig. 3.

DISCUSSION

Although DFT produces a similar band structure to that from GW, Fig. 1 shows that there are notable differences between the two, even after correcting DFT's band-gap to match GW's. The influence of deformation potential inputs on the deformation scattering rate can be clearly seen in Fig. 2. Fig. 3 demonstrates that empirical models such as VFF, although computationally inexpensive, have major differences from those computed from more fundamental methods. As seen in Fig. 4, the effect of different constant values chosen for the phonon deformation potentials shows a strong sensitivity of the impact ionization coefficient on the assumed deformation potentials, demonstrating the need for k-vector dependent deformation potentials from accurate phonon dispersion inputs.

CONCLUSION

Using inputs calculated from first principles methods can help to compensate for the shortage of experimental data available for newer materials such as UWBG semiconductors. More traditional approximations, such as constant deformation potential values and empirical electronic and phonon dispersions, aren't sufficiently accurate for predicting UWBG material ionization coefficients. GW electronic structures and DFPT phonon dispersions help to produce more accurate ionization coefficients, but it is important to compare the various choices for pseudopotential functions.

ACKNOWLEDGMENT

This work was supported as part of ULTRA, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES).

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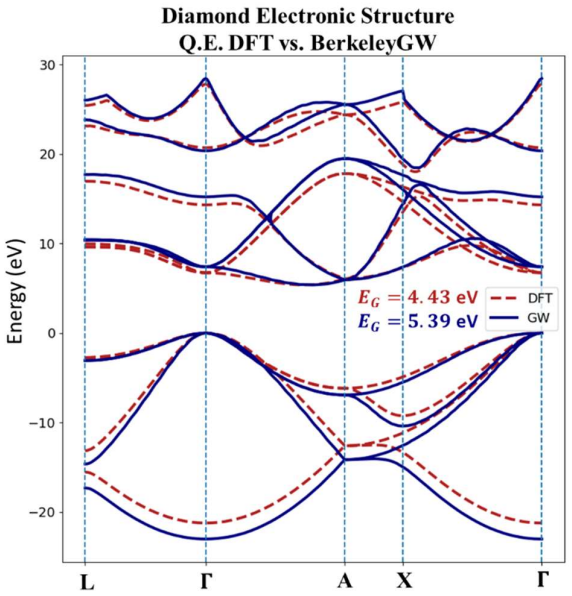

Fig. **1**. Electronic structures computed from Density Functional Theory (DFT) using Quantum Espresso (red) and from GW using BerkeleyGW (blue). The DFT electronic structure conduction bands are shifted to match the GW-calculated band-gap (values shown on figure).

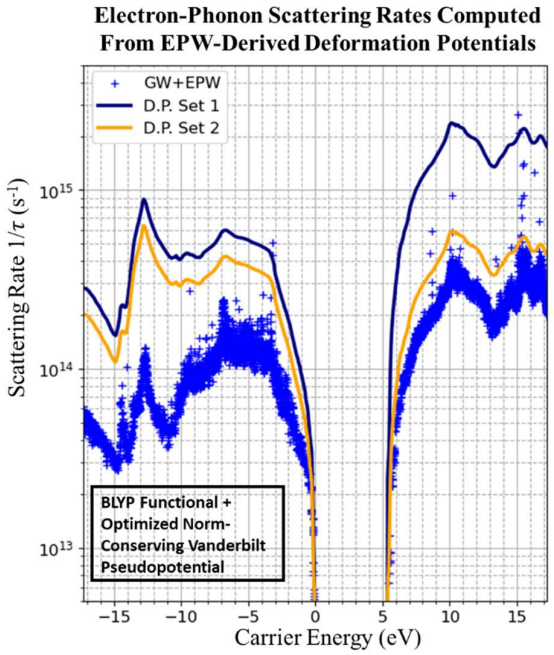

Fig. 2. Electron-Phonon scattering rates computed from EPW-derived deformation potentials, using GW energies and wavefunctions as input (blue). The phonon band structure is computed using DFPT in Quantum Espresso. Both sets of points calculated using a BLYP functional and optimized norm-conserving Vanderbilt pseudopotential input.

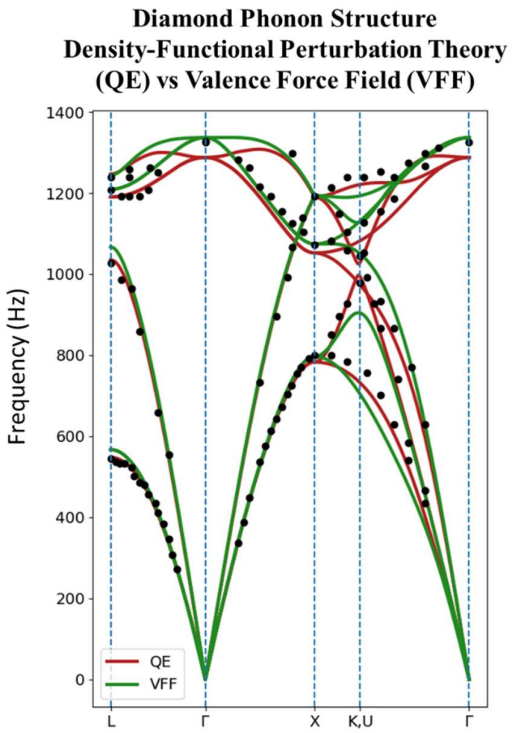

Fig. 3. Phonon dispersions computed from Density Functional Perturbation Theory (DFPT) using Quantum Espresso (red) and from Valence Force Field (VFF) model (green). The DFPT phonon structure is computed using a BLYP functional and optimized norm-conserving Vanderbilt pseudopotential input.

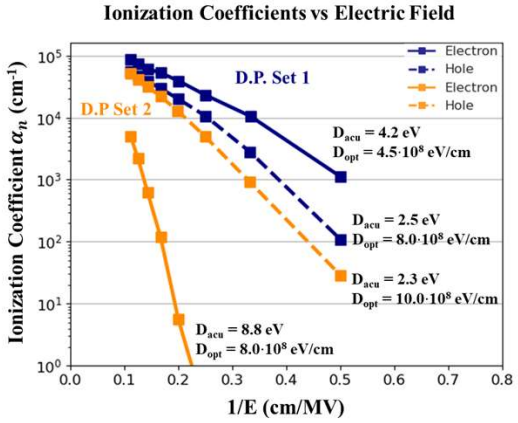

Fig. 4. Impact ionization coefficients from Monte Carlo simulations using two different sets of constant deformation potentials as input. The blue curves use the deformation potential scattering rate (shown in Fig. 2) computed from D.P. Set 1 (inset), and the orange curves use the rate computed from D.P. Set 2 as input. The resulting ionization coefficients are highly influenced by the choice of deformation potential values.