Full Band Monte Carlo Simulation of Impact Ionization in Wide Bandgap Semiconductors Based on *Ab Initio* Calculation

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***Abstract*—A full band Monte Carlo simulation based on *ab initio* calculations is presented to investigate high-field carrier transport characteristics. The band structure and the impact ionization rate of wide bandgap semiconductors are calculated based on a quasiparticle selfconsistent *GW* method. Then, we demonstrate the full band Monte Carlo simulation in diamond to investigate the electron and hole ionization coefficients. It is shown that the estimated breakdown fields are in good agreement with the experimental data of n^+p^- one-sided abrupt junctions with the acceptor density less than 10^{17} cm^{-3}.**

I. Introduction

Wide bandgap semiconductors are greatly attractive for the application of next generation power devices. However, completeness of the device simulation models is still poor compared to, e.g., Si, which are the issues for device design and optimization with the effective use of TCAD. In order to overcome such situation, *ab initio* calculation is considered to be a promising approach to predict unknown parameters. For example, in the case of power device simulation, impact ionization is one of the most essential phenomena to be accurately modeled, because the avalanche breakdown tolerance is one of the key factors determining the device performance. Thus, in this study, we are investigating the impact ionization processes using a full-band Monte Carlo (FBMC) simulator based on the state-of-the-art *ab initio* calculations. In this work, we calculate the band structure and impact ionization rate of wide bandgap semiconductors (SiC and diamond) using a hybrid quasiparticle selfconsistent *GW* (QSGW) method [1], and the results are compared to previous calculations based on the empirical pseudopotential method. Then, we implement the results for diamond into the FBMC simulator to investigate their validity through the calculation of high-field carrier transport properties as well as the avalanche breakdown field [2].

II. Calculation of Band Structure and Impact Ionization Rate with QSGW Method in Si, SiC, and Diamond

In this work, the electronic band structure to be implemented into the FBMC simulator was computed based on a quasiparticle selfconsistent *GW* (QSGW) method using the ecalj code [1]. Although the *ab initio* calculation method based on the local density approximation (LDA) is now frequently used, its application to FBMC simulation is not necessarily appropriate due to its deficiency in the prediction of band properties, such as energy gap and effective mass. On the other hand, QSGW method systematically slightly overestimates the band-gap energy, but a hybrid QSGW method [3] is effective to precisely reproduce the experimental band gap energy. For example, Figure 1 shows the calculated band structure of bulk 4H-SiC; by mixing 79.5% of QSGA and 20.5% of LDA, the experimental gap energy of 3.26 eV [4] was obtained, and then the other band parameters were also confirmed to be reasonable as shown in TABLE I.

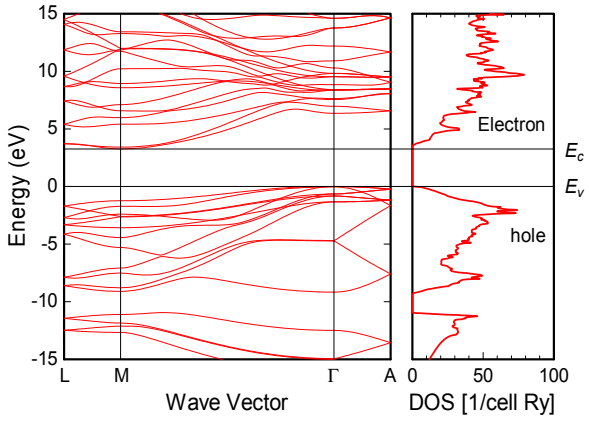

Fig. 1. Band structure and density of states of bulk 4H-SiC calculated by the hybrid QSGW method.

TABLE I. Direct Band Gap Energies and Effective Masses of 4H-SiC compared with the experimental data [5,6].

	Direct band Gap energy at symmetry points (eV) [5]		Effective mass at conduction band bottom (m_0) [6]	
	Γ	M	$m^*_{M\Gamma}$	m^*_{MK}
Experiment	6.18	4.56	0.58	0.31
This Work	6.36	4.50	0.53	0.28

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Figure 2 shows the band structure of diamond compared to that obtained from the empirical pseudopotential method with parameters determined to fit the measured transition energies related to relatively low carrier energy region (−15 eV ~ 15 eV) [7]. In this area, the results of both methods are similar, but they deviate from each other with distance from the band gap. For example, the valley-like density of states (DOS) confirmed in *ab initio* band structure around ~19 eV (or, ~13.5 eV from the top of the conduction band) has an essential impact on the high-field transport properties.

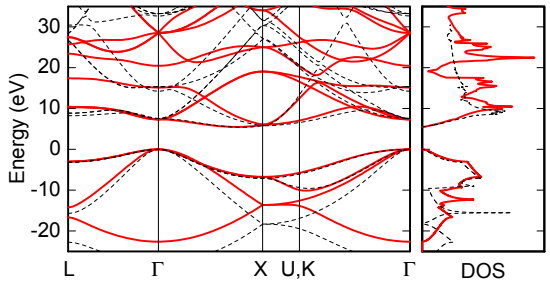

Fig. 2. Band structure and density of states in bulk diamond calculated by the hybrid QSGW method [3] (solid lines) compared with the result based on the empirical pseudopotential method [7] (dashed lines).

Impact ionization is an important mechanism to determine the high-field carrier transport properties, such as breakdown field, and its rate can be calculated straightforwardly with the QSGW method from the quasiparticle width in the *GW* approximation [8]. Figure 3 shows the calculated impact ionization rates in Si, 4H-SiC, and diamond plotted together with the previous results obtained by the empirical pseudopotential method and fitted to the modified Keldysh formula. In the case of Si, the *ab initio* result shows good agreement with the previously reported rates for electrons [9] and holes [10] in low carrier energy region. On the other hand, the present results for 4H-SiC and diamond are much smaller than the previously reported values [7,11]; the impact ionization rates from the QSGW calculation tends to be smaller than the empirical pseudopotential based results in particular in the high energy region [8].

III. Full Band Monte Carlo Simulation in Bulk Diamond

Diamond is one of the most promising materials for power devices due to its attractive properties such as wide band gap, high mobility, and high thermal conductivity. Despite great expectations for the high avalanche breakdown tolerance, understanding of hot carrier transport in diamond is still not enough. So far, e.g., a FBMC simulation [7] was performed for electrons based on the empirical pseudopotential band calculation, but it has been recently pointed out that the calculated ionization coefficient significantly underestimates the experimental breakdown fields [12,13].

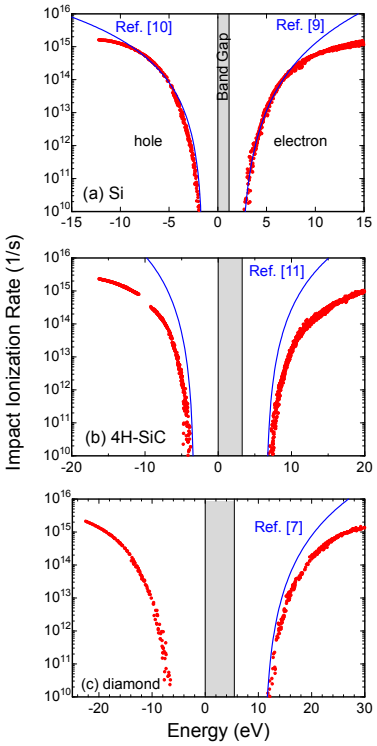

Fig. 3. Calculated impact ionization rates in (a) Si, (b) 4H-SiC, and (c) diamond plotted as a function of the electron energy measured from the top of the valence band. The results obtained with the QSGW method (dots) are compared to the rates given in previous papers (lines) [7,9-11].

We hence investigated the impact ionization processes using a FBMC simulator for electrons and holes in diamond based on the state-of-the-art *ab initio* calculations [2]. The concept of the simulation framework is presented in Fig. 4. In this simulator, the *k*-space is discretized into equal grids (Γ-X in the first Brillouin zone was divided into 40 grids), and the *E*-*k* relationship (4 valence bands and 12 conduction bands) is stored as a look-up table. The electronic band structure and impact ionization rate were obtained with the hybrid QSGW method, while lattice-dynamical properties were computed based on density functional perturbation theory within the LDA using the Quantum ESPRESSO code [14], and then the EPW code [15,16] was employed to calculate the carrier-phonon scattering rates.

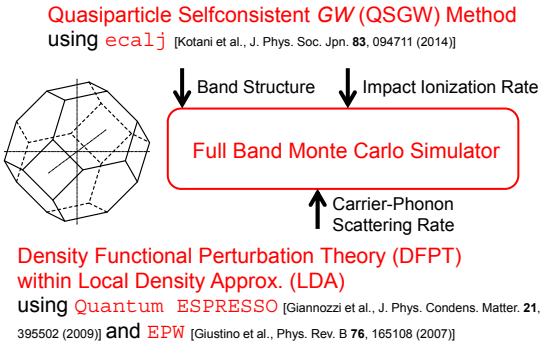

Fig. 4. Schematic view of the cocept of FBMC simulation performed in this study.

Figure 5 shows the carrier-phonon scattering rates plotted as a function of energy. The longitudinal acoustic (LA), transverse acoustic (TA), and optical phonon scattering rates calculated by the EPW code are shown in Fig. 5 (a), while the electron-phonon scattering rates used in [7], where the deformation potentials were determined by fitting procedure to reproduce the measured electron drift velocity [17], are plotted in Fig. 5 (b). Note that a large difference between the two approaches is found especially in the magnitude of the optical phonon scattering rate. However, its impact on the simulated velocity-field curve is not significant; as shown in Fig. 6, both results exhibit good agreement with the experimental data [18,19].

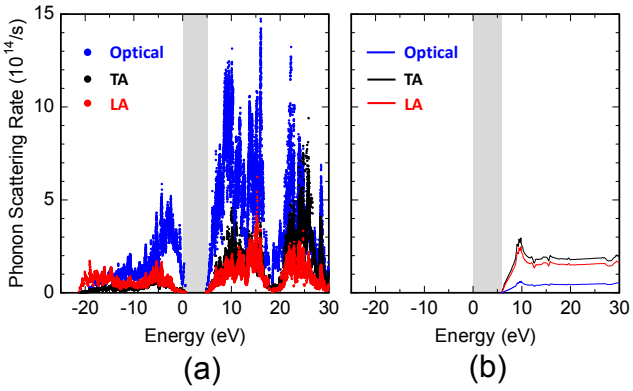

Fig. 5. Carrier-phonon scattering rates plotted as a function of electron energy measured from the top of the valence band. The results calculated by the *ab initio* calculation is shown in (a), while the rates used in [7], where the deformation potentials were determined by fitting procedure, are plotted in (b).

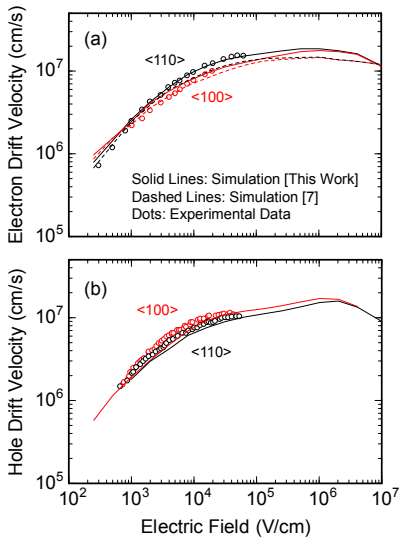

Fig. 6. Drift velocity for (a) electrons and (b) holes in diamond at 300 K plotted as a function of the electric field along <100> and <110> directions. Experimental data (electrons: [18], holes: [19]) are also plotted with symbols.

However, in contrast to the case of the drift velocity, a large discrepancy was found in the ionization coefficient between the two approaches as shown in Fig. 7. It was also found that (i) the hole ionization coefficient α_p is larger than α_n due to smaller hole-phonon scattering rate than electron's [20], and (2) α_n and α_p exhibit negative temperature coefficients, but are less sensitive compared to, e.g., Si due to the larger optical phonon energy.

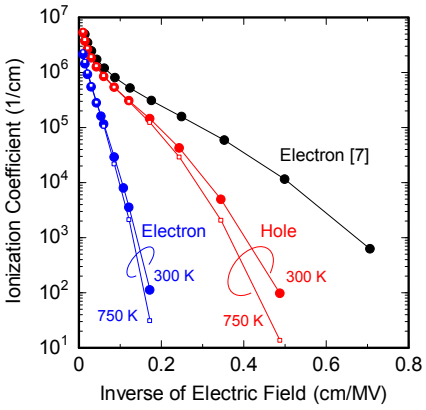

Fig. 7. Ionization coefficient for electrons (blue) and holes (red) in diamond simulated under homogeneous electric field along <100> direction at 300 K (closed dots) and 750 K (open dots). The restuls based on the empirical pseudopotential method are plotted with black dots.

Figure 8 compares the electron energy distributions. The previous empirical approach underestimated the phonon scattering rate in high-energy regime (mainly for optical phonons), and thus the electrons can easily run away from the phonon scattering. On the other hand, in this work, the larger phonon scattering rates prevent the electron acceleration, and also, under very large electric field (~20 MV/cm), the valley-like DOS confirmed in Fig. 2 blocks the electron heating.

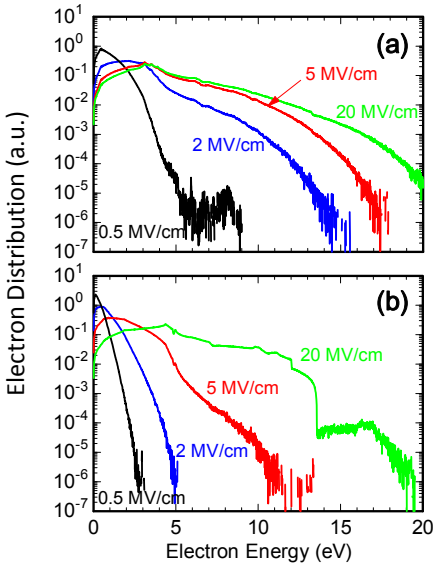

Fig. 8. Energy distribution of electrons in diamond at 300 K under various homogeneous electric fields along <100> direction. The electron energy is measured from the bottom of the conduction band. The results simulated based on (a) the empirical pseudopotential method [7] and (b) the *ab initio* calculations are compared.

Finally, the breakdown field (F_{BD}) of one sided abrupt n^+p^- junction were estimated as a function of the doping density N_A in the p^- region were estimated as Fig. 9 using α_n and α_p shown in Fig. 7 according to the calculation method given in [12,13]. For comparison, the ever reported experimental data obtained measuring Schottky barrier diodes are also plotted based on [12,13]; note that the present result well reproduced the experimental trends for diamond [21-24], except the record-high F_{BD} of Landstrass *et al.* [25]. The physical origin for this discrepancy still remains unclear. Recently, several studies questioned the accuracy of the DFPT-based electron-phonon matrix elements when obtained with local functionals such as LDA [10,26]. However, to obtain F_{BD} = 20 MV/cm at $N_A = 10^{18}$ cm^{-3}, *e.g.*, much larger hole-phonon scattering rate had to be used to suppress the hot hole generation.

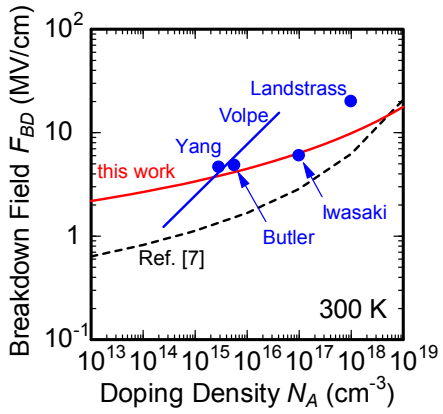

Fig. 9. Estimated avalanche breakdown field of a uniformly doped one-sided abrupt junction of diamond plotted as a function of N_A with various experimental data summarized by Hiraiwa et al. in [12,13]. The results of this work are represented by red solid line, which were calculated with α_n and α_p given in Fig. 7, while those based on the empirical pseudopotential method [7] is shown by dashed lines.

IV. Conclusion

We have presented a full band Monte Carlo simulation based on *ab initio* calculations, and investigated the high-field transport in diamond. The obtained breakdown field exhibited good agreement with experimental data of n^+p^- one-sided abrupt junctions with $N_A < 10^{17}$ cm^{-3}. It has been demonstrated that the present computational approach is extremely useful as a way to predict the electron device properties for which no definite material parameters are available.

Acknowledgment

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