Impact Ionization in Monoclinic $\beta$-Ga$_2$O$_3$

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We report a theoretical investigation of extremely high field transport in an emerging wide-bandgap material $\beta$-Ga$_2$O$_3$ from first principles. The signature high-field effect explored here is impact ionization. Interaction between a ground-state electron and an excited electron is computed from the matrix elements of a screened Coulomb operator. Maximally localized Wannier functions (MLWF) are utilized in computing the electron-electron self-energy. A full-band Monte Carlo (FBMC) simulation is carried out incorporating the impact ionization rates, and electron-phonon scattering rates. Possibility of room temperature Bloch oscillations is predicted in bulk $\beta$-Ga$_2$O$_3$. This work brings out valuable insights on the impact ionization coefficient (IIC) of electrons in $\beta$-Ga$_2$O$_3$. The isolation of the $\Gamma$ point conduction band minimum by a significantly high energy from other satellite band pockets play a vital role in determining ionization co-efficients. IICs are calculated for electric fields ranging up to 8 MV/cm for two different crystal directions. A Chynoweth fitting of the computed IICs is done to calibrate ionization models in device simulators.

I. INTRODUCTION

Wide-bandgap semiconductors are attractive for high voltage and high-power electronics, and UV optoelectronic applications. A recently emerged material $\beta$-Ga$_2$O$_3$ has gained a lot of attention due to its immense potential in both electronics and photonics. High breakdown voltage MOSFETs, Schottky diodes, and deep UV photodetectors are experimentally demonstrated. Well developed bulk and thin film growth techniques make this material a strong candidate for future applications. Accurate $n$-type doping and the difficulty in $p$-type doping make electrons the dominant carriers in this material. Electronic structure, optical absorption, and lattice dynamical calculations in this material have been reported in last few years. Theoretical investigation of electron transport in this material is crucial to augment the experimental advancements. There have been a few low-field transport calculation reports in this material revealing that the long-range polar optical phonon (POP) electron-phonon interactions (EPI) limit the electron mobility. Recently, we reported a high-field transport calculation including full-band EPI to predict velocity-field curves in this material for an electric field up to 0.4 MV/cm. However, as the electric field is further increased, interband transitions and electron ionization become important. Indeed, in power devices the electric field reaches up to several MV/cm and the resulting ionization of electrons could lead to breakdown of devices. An empirical estimate of critical breakdown electric field in $\beta$-Ga$_2$O$_3$ based on bandgap is reported. We have previously reported on the impact ionization coefficient in $\beta$-Ga$_2$O$_3$ using a simple semi-classical calculation. But, given the exponential sensitivity of the ionization coefficients on the electric field it is crucial to carry out a much rigorous calculation from first-principles. Proper understanding of electron-electron interaction is the key to probe impact ionization.

Recent advancements in electronic structure and lattice dynamics calculations motivates accurate model development for non-equilibrium carrier dynamics. There have been several reports on first-principle EPI calculation and subsequent carrier lifetime estimation with high accuracy. There are reports on the high-field transport based on empirical pseudo-potential models under rigid-phonon approximations that include impact ionization. Conventionally, deformation potential based theories for EPI and a Keldysh empirical ionization model are common practice in Monte Carlo simulations. Here, we explore impact ionization starting from density functional theory (DFT) under local density approximation (LDA). The uniqueness of this work is that we utilize a maximally localized Wannier basis to calculate electron-electron interactions (EEI). While maximally localized Wannier functions (MLWFs) have been used in EPI formulation with high accuracy, they have not been used to calculate EEI to the best of our knowledge. The method we describe here is expected to provide sufficient accuracy within reasonable computational requirements. Using these EEI calculations, electron-electron self-energy is obtained using Fermi-Golden rule. Full-band Monte Carlo (FBMC) simulation is carried out to extract the impact ionization co-efficients (IICs). The IICs are fitted to a Chynoweth model to help calibrate device simulators. While this work focuses on EEI, the description of the EPI calculation could be found in our previous work. First, we discuss the theory and methods of the EEI and IIC calculations followed by the results obtained for $\beta$-Ga$_2$O$_3$.

II. THEORY AND METHODS

The Coulombic interaction between two Bloch electronic wavefunctions can be expressed by the matrix el-
elements $\langle \Psi_{nk} | V_q | \Psi_{mk-q} \rangle$ where $V_q$ is the interaction potential and $\Psi$ s are the electronic eigen functions with proper wave-vector and band indices. Using cell-periodic Bloch functions, $|nk\rangle$, we can write the matrix elements as

$$M_q = \langle nk | V_q e^{-iq \cdot r} | mk-q \rangle$$

Now using maximally localized Wannier(MLW) functions \cite{Marzari97a}, the cell-periodic part of the electronic wavefunctions can be written as $|nk\rangle = \frac{1}{V} \sum_{mR_e} U_{k}^{\dagger} R_{e}^{\dagger} U_{k} R_{e} | mR_e \rangle$, where $|mR_e\rangle$ is an MLW function centered at $R_e$. $U_{k}$ is the gauge-transforming unitary matrix that rotates the Bloch functions to the MLW basis. Utilizing the orthonormality relation of the Wannier functions and under a small $q$ limit, Eq. 1 can be rewritten as

$$M_q = U_{k}^{\dagger} V_q U_{k-q}$$

$V_q$ typically has a $\nabla^2$ divergence and hence the small $q$ limit is justified. However, this is true only under a weak screening limit. We take into account screening of the Coulombic interaction by considering a dynamic polarizability (frequency dependent) \cite{Kohn86} under a long-wavelength limit $q \to 0$. For screening by free carriers we use a Debye wave-vector calculated under non-degenerate carrier conditions. The screened Coulombic potential, in atomic units, has the form $V_q = \frac{1}{\Omega} \sum_{i} \frac{\epsilon(\omega)}{q^2 + qD^2} qD$, where $\Omega$ is the unit cell volume, $\epsilon(\omega)$ is the dynamic dielectric constant, and $qD$ is the Debye wave-vector.

The advantage of the proposed approach of using MLW functions for EEI is the ability to obtain a very fine sampling of the Brillouin zone in calculating the interaction terms. The $U_k$ elements are the eigen functions of the interpolated Kohn-Sham(KS) Hamiltonian. First the $U_k$ matrices are calculated on the coarse mesh followed by a Fourier interpolation of the KS Hamiltonian in the Wannier gauge, which will give the $U_k$ matrices on a finely sampled Brillouin zone. Impact ionization is a two electron process which involves relaxation of a hot electron in the conduction band and excitation of a valence electron into the conduction band. Using the EEI expression describe above the impact ionization interaction term can be written as

$$M_q^{(1)} = U_{k}^{\dagger} U_{k}^{\dagger} V_q U_k q U_{k+q}$$

Here $k$ is the wave-vector of the final-state of the electron that gets excited from the valence band and $k'$ is the wave-vector of the of the conduction band hot electron after relaxation. Next, the electron-electron self-energy is calculated using Fermi-Golden rule enforcing the energy conservation $\delta(E_{mk-q} + E_{nk+q} - E_{nk} - E_{n'k'})$ where $E_{nk}$ is the KS eigen value of the $n^{th}$ band at a wave-vector $k$. To correct the mean-field (LDA) estimated bandgap we shift the conduction band energies to match the experimental bandgap. It is noted that the mean-field estimated wave-functions are close to the actual quasiparticle wavefunctions \cite{BerkeleyGW}, and hence the formulation of $U_k$ starting from LDA estimated wave-functions is justified.

The FBMC simulation takes into account EEI and EPI. The IIC ($\alpha$) is defined as the reciprocal of the mean free path traversed by an electron before creating an ionization. The FBMC scheme outputs the generation rate ($G$) of electrons per unit time. We extract IIC($\alpha$) from the generation rate ($G$) using the relation $G(F) = \alpha(F) v_d(F)$, where $v_d(F)$ is the drift velocity for an applied electric field $F$ which is calculated in the FBMC simulation. While the details of EPI could be found in our previous reports \cite{Sugiyama92, Sugiyama93}, here we describe the methodology in a few sentences. Using density functional perturbation theory \cite{Marzari97c}, the phonon eigen values, displacement patterns, and EPI elements are calculated on coarse mesh. Next, the Wannier-Fourier interpolation \cite{Marzari97b, Marzari97c} is carried out using a semi-coarse interpolation method (see \cite{Baroni99}) to calculate the EPI elements and the phonon dynamical matrices. Long-range POP scattering is calculated separately following \cite{Baroni99}.

### III. RESULTS AND DISCUSSIONS

First, we carry out the density functional theory (DFT) calculations on $\beta$-Ga$_2$O$_3$ unit cell \cite{Sugiyama92} under LDA using norm-conserving pseudopotentials \cite{Baroni99} in Quantum ESPRESSO \cite{QE2013}. The Brillouin zone is sampled with Monkhorst-Pack \cite{Monkhorst76} grid of $8 \times 8 \times 4$ with an energy cut-off of 80 Ry to truncate the reciprocal vectors. The $\beta$-Ga$_2$O$_3$ conventional unit cell is shown in Fig. 1(a) and the interpolated KS eigen values are shown in Fig 1(b) for two reciprocal crystal directions. The inset in Fig. 1(b) shows the BZ with the corresponding reciprocal directions. To obtain the screening element, $\epsilon(\omega)$, we use the full-frequency epsilon calculation as implemented in BerkeleyGW \cite{BerkeleyGW}.

We compute the ionization rates using the theory described in the previous section. The electron-electron self-energies for conduction bands 5 and 6 are shown in Fig. 1(c) along the two reciprocal vector directions. In the Monte Carlo scheme ionization rates are included only from bands 5 and 6 since the lower bands (bands 1-4) do not have energy states high enough to cause ionization. It is noted that band 4 has some energy states away from the zone center that have energy higher than the bandgap but there computed ionization rates (not shown) are much smaller than the EPI scattering rates. It could be seen that the ionization rates are much higher near the zone center compared to the zone edges. This peculiarity arises from the isolation of the conduction band minimum at the $\Gamma$ point by a significantly high energy difference. To be more specific, the electrons near the zone edge in bands 5 and 6 which have energies higher than the bandgap cannot ionize as there are no available final states. The long-range nature of the interaction prohibits a zone edge electron to release enough energy (> bandgap) and end up near the zone center. Hence the ionization rates mediated by the zone edge hot electrons are significantly lower than that by zone center electrons.
FIG. 1. (a) The monoclinic lattice (visualized by Vesta [35]) with the Cartesian directions used in this work. The crystal lattice directions are also shown. The angle between $c$ and $c^*$ is 13.83° [41]. Larger atoms are Ga while smaller ones are O (b) The Wannier interpolated bandstructure in two reciprocal directions. The mean-field computed excited-state eigen values are scissor shifted to match experimental bandgap. The blue and green arrows show the two possible EEI mediated transitions taken in our calculation. (inset) the first BZ ((visualized by XCrySDen [36])). (c) The imaginary part of the computed electron-electron self-energy using MLWF and Fermi-Golden rule for two conduction bands.

Fig. 2 shows the contributions of the individual electronic bands in impact ionization. It could be seen that the ionization rate follows Keldysh power law [29] near the ionization threshold which is slightly above 5 eV.

Next, we carry out the FBMC simulation using our in-house codes. The FBMC scheme initializes the ensemble of electrons thermodynamically after which the electric field is turned on. Trajectories of the electrons are formed in reciprocal space stochastically by using the electron-phonon scattering rates, and electron ionization rates. Six conduction bands are taken into account in the FBMC simulation. We ran the FBMC simulation for electric fields ranging from 1 MV/cm to 8 MV/cm.

Fig. 3(a) shows the transient electron dynamics under an applied electric field of 2 MV/cm. The oscillations that are observed initially result from the reflection of electrons at Bragg planes which are subsequently suppressed out due to EPI. This oscillation, often known as Bloch oscillation (BO), is experimentally observed in superlattices [43] at room temperature. However, in $\beta$-Ga$_2$O$_3$, the satellite valleys occur at an energy comparable with the zone edge maxima of the first conduction band. Hence the onset of intervalley scattering occurs only near the zone edge where the reflection (reversal of electronic group velocity) is also likely to onset. The time-period of oscillation ($T_B$) in Fig. 3(a) matches well with the analytically calculated BO time-period $T_B = \hbar/eFd$, where $d$ is the distance of the Bragg plane from the zone-center further confirming the origin of the oscillations. However, for further certainty on whether BO is actually realizable in $\beta$-Ga$_2$O$_3$ at room temperature, one needs to take into account interband tunneling which is beyond the scope of this work.

Fig. 3(b) shows the occupation of the bands as the electric field is increased in two different directions. In our calculation the interband transitions occur only via short-range EPI and long-range EEI. Fig. 3(c) shows the calculated IICs along two different directions. The anisotropy in the IIC is attributed to the anisotropy in EEI which in turn originates from the anisotropy of the higher conduction bands (bands 5 and 6 in this case) even near the $\Gamma$ point as seen in Fig. 1(c). For comparison, the calculated IIC is less than that computed in GaN [28] for a similar range of electric fields which indicates a higher avalanche breakdown field for $\beta$-Ga$_2$O$_3$.

Finally, to help facilitate device simulation, we perform a Chynoweth fitting of the calculated IIC. The Chynoweth model [44] formulates the IIC as $\alpha(|F|) = ae^{-b/|F|}$, where $a$ and $b$ are the fitting parameters. In order to account for the anisotropy in IIC, we provide two sets of the parameters for two different directions—$a_z = 0.706 \times 10^6$ V/cm, $b_z = 2.1 \times 10^7$ V/cm, $a_x = 0.79 \times 10^6$ V/cm.
TB FZ = 2 × 10^8 V/m

FIG. 3. (a) The Bloch oscillations under an electric field 2 × 10^8 V/m. The time period of the oscillation matches well with the analytical BO time period (see text for details). (b) The fractional band population as a function of the electric field from FMBC simulation. Circles represent the case when the applied electric field is in x direction, while squares represent the same for z direction. (c) Computed IIC for two different Cartesian directions.

IV. CONCLUSIONS

We computed ionization rates and co-efficients in β-Ga_2O_3 from first-principles. FBMC simulation is done for a wide-range of high electric fields along two different directions. We predicted the possibility of Bloch oscillations at room temperature in this material. IIC is fitted to an empirical Chynoweth model to calibrate device simulators. A hypothetical estimate using the computed Chynoweth parameters predicts avalanche breakdown field to be higher than the existing empirical value of 8 MV/cm.

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