Full-band Monte Carlo simulation of two-dimensional electron gas in (Al$_x$Ga$_{1-x}$)$_2$O$_3$/Ga$_2$O$_3$ heterostructures

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β-Gallium Oxide (Ga$_2$O$_3$) is an extensively investigated ultrawide-bandgap semiconductor for potential applications in power electronics and RF switching. The room temperature bulk electron mobility ($\sim$200 cm$^2$V$^{-1}$s$^{-1}$) is comparatively low and is limited by the 30 phonon modes originating from its 10-atom primitive cell. The theoretically calculated saturation velocity is 1.2-10$^7$ cm$^{-1}$s$^{-1}$ which is comparable to GaN. The high field electron transport in the 2DEG is explored in this work based on the first principles calculated parameters. A self-consistent calculation on a given heterostructure design gives the confined eigenfunctions and eigenenergies. The intrasubband and the intersubband scattering rates are calculated based on the Fermi’s golden rule considering LO phonon-plasmon screening. The high field characteristics are extracted from the full-band Monte Carlo simulation of heterostructures at 300 K. The motion of electrons in the 2DEG and the bulk is treated through an integrated Monte Carlo program which outputs the steady state zone population, transient dynamics and the velocity-field curves for a few heterostructure designs. The critical field for saturation does not change significantly from bulk values, however an improved peak velocity is calculated at a higher 2DEG density. The velocity at low 2DEG densities is impacted by the antiscreening of LO phonons which plays an important role in shaping the zone population. A comparison with the experimental measurements is also carried out and possible origins of the discrepancies with experiments is discussed.

I. INTRODUCTION

β-Ga$_2$O$_3$ is a promising wide-bandgap semiconductor material known for its potential applications in high voltage power electronic[9][10] and high power radio frequency (RF) switching[11][12]. The power electronics application comes from its large Baliga’s figure of merit (BFoM = $\epsilon$µ$E_s^2$) resulting from its wide bandgap (4.8 eV)[13][14] and a very high estimated breakdown field ($E_b = 8$ MVcm$^{-1}$)[15]. The RF performance of a material is characterized by its Johnson’s figure of merit, given by $JFoM = E_bv_s/2\pi$, where $v_s$ is the saturation velocity, which in turn is limited by the low field electron mobility. The bulk mobility in the corresponding devices is low, due to dominant multiple polar optical modes present at 300 K[16][17], which is shown to be improved in the 2DEG of AlGa$_2$O$_3$/Ga$_2$O$_3$ heterostructures in our previous work[18]. There are several experimental measurements on modulation doped transistor of AlGa$_2$O$_3$/Ga$_2$O$_3$ reporting low field electronic mobility at low and room temperature[19][20]. Zhang et al[21] recently reported velocity-field characteristics of such heterostructures at 50 K and the corresponding low field mobility and saturation velocity are found to be ~1500 cm$^2$V$^{-1}$s$^{-1}$ and 1.1×10$^7$ cm$^{-1}$s$^{-1}$ respectively. The high field electron transport in a bulk material has been reported previously[22]. Yan Liu et al[23] recently reported Monte Carlo based velocity-field characteristics of unintentionally doped heterostructures based on analytically calculated scattering rates. However, there are no reports for the 2DEG which takes into account the first principles calculated full band electron-phonon interaction elements. It is of high interest to incorporate those parameters in order to completely understand the behaviour of heterostructures when subjected to high field to fully take the advantage of such devices.

A complete ab-initio study of β-Ga$_2$O$_3$ is very challenging as compared to other wide-bandgap materials like GaN due to it’s low crystal symmetry and large primitive cell size. However, a full band Monte Carlo (FBMC) investigation is required with the inclusion of true electron-phonon interaction (EPI) elements to capture the band anisotropy as well as non-parabolic effects.

We discuss a basic flow of methods used for our Monte Carlo simulation in the next section. The calculation starts with first principles calculation on electronic band structure and phonon dispersion followed by short range and long range electron phonon interaction element calculation. This is followed by finding a self-consistent solution of the device in consideration which outputs necessary quantum well parameters required for the scattering rate calculation. We then discuss the methods and equations used for 2D & 3D scattering rate calculation followed by a discussion on different scattering rates variation.

In the third section, we discuss the FBMC simulation along with different steps involved in the process. We discuss the equilibrium distribution of an ensemble of electrons when no field is applied. Next, we discuss the normalized scattering rate needed to select a random scattering process during the simulation. Finally, in this section, we discuss the final state election methods and their implementation for different scattering mechanisms and transport regime.

The results extracted from FBMC simulation are discussed in the third section. We discuss the zone population at different fields in energy and k-space. This is followed by a discussion on transient dynamics and velocity field characteristics for a few cases. We also present a comparison with an experimental device and discuss the possible reasons of discrepancies observed.
We finally conclude our work in the fifth section with a quick look on important results and discuss any suggestions for improvements in current heterostructure devices to help the experimental community.

II. METHODOLOGY

Fig.1 shows a basic flow chart of the calculations involved in the high field electron transport simulation. The process starts with calculating the \textit{ab-initio} parameters from well established density function theory (DFT) and density functional perturbation theory (DFPT) calculations using existing tools and techniques. This gives the electronic band structure, phonon dispersion and electron-phonon interaction elements used later scattering rate calculations and in FBMC simulation. This is followed by finding self-consistent solution of the heterostructure in consideration from which the 2DEG and the device parameters are extracted. The earlier two steps provides us with the necessary parameters for the scattering rate calculation which is the next step in the process. The last step is to run the FBMC simulation until a convergence in an observable is achieved. The FBMC involves three main subprocesses: electron drift, randomly selecting a scattering even and the corresponding final state selection. We next provide a brief description of first principles, self-consistent and the scattering rate calculation. The FBMC is, however, discussed in the next section to provide a better understanding of the method given its computational complexity.

A. First principles calculations

The electronic band structure, as shown in fig[2], is first calculated and Wannier interpolated on a fine k-grid using Quantum Espresso\textsuperscript{34} followed by Wannier90 package\textsuperscript{35}. A 80×80×80 k-mesh is used for the electrons in the 3D regime and a more denser k-mesh of 200×1×200 is used for the electrons in the 2D regime. The 2DEG is assumed to be confined in the cartesian y-direction. The 2D-bandstructure in fig[2] is plotted in x-z cartesian space and the 3D-bandstructure in fig[2] is shown along Y(0,0,5,0) and Z(0,0,0,5) reciprocal space directions. Only first two conduction bands are taken into account following a previous work\textsuperscript{33} on a bulk system where the distribution at moderately high fields drops rapidly after ∼2 eV. The conduction band minimum is fairly isotropic with electron effective mass in the range (0.27-0.3)m\textsubscript{e}. The non-parabolicity in the band structure starts to appear at higher energies. It is important to point out that the first satellite val-
The long range nature of polar optical phonons (POP) is properly captured with a very dense grid of $40 \times 40 \times 40$ covering just the 40% of the full brillouin zone. In order to incorporate the dynamic screening of POP through 2D-plasmons, the electron - LO phonon interaction elements are calculated using Fröhlich interaction following our earlier work\textsuperscript{25,26} In addition, the matrix elements are required to be stored for each $k$, each $q$ and for every mode $\nu$ for later use. POP modes do not mediate any inter-band scattering and are $k$ independent due to their long range nature (small $q$) and hence are much easier to handle. The POP EPI elements are calculated separately as described in the next section, with first principles parameters such as LO-TO frequencies, dielectric tensor ($\varepsilon_{\infty}$) and displacement vectors as input extracted from DFT and DFPT calculations. The pure LO modes corresponding to each $q$ are calculated by diagonalizing the DFPT computed dynamical matrix at $\Gamma$ point with macroscopic polarization added.

The short range electron-phonon interaction elements (Acoustic and Non-polar optical phonon) are calculated on a $40 \times 40 \times 40$ q-grid in the entire brillouin zone using EPW package\textsuperscript{27} The non-polar EPI elements are calculated using EPW package through Wannier interpolation of matrix elements on a coarse mesh. For low energies, the contribution to the non-polar matrix elements coming from the overlap integral of the periodic part of the Bloch wavefunction becomes 1 due to spherical and isotropic bands. This enables us to directly use the 2D scattering rate equation. For higher energies, when the electron is in the bulk, there are no such approximation as the corresponding matrix elements are highly anisotropic and must be considered with a proper care. For non-polar EPI elements, the initial and final state bands are also stored, exponentially increasing the memory requirement. The idea to reduce the space requirement is to only store those matrix elements where energy-momentum conservation is satisfied as the rest will be anyway rejected during the final state selection in the Monte Carlo technique (discussed later). This is done with a little modification in the EPW code. In order to minimize RAM requirements, the non-polar matrix elements are divided and stored in multiple files and read through I/O process during the simulation. This is still computationally intensive as during a parallel run, multiple cores could access the files at the same time and abruptly increase the RAM requirement. This is optimized through trading off the number of files as more number number of files would take more time to read which is again not desired. Note that total memory requirement (main memory) remains the same with number of files.

B. Self-consistent solution

A heterostructure device, as shown in the inset of fig.3(a), is used as a reference with 20% aluminum concentration in the alloy and impurities doped at 3 nm (spacer thickness) away from the interface. However, the spacer thickness is adjusted to 4.5 nm to provide a fair comparison with the experiment. Table I shows a list of material parameters used in our simulation. As seen in the fig.3(a), a 2DEG is formed at the interface, confined in a quantum well. The delta doping is adjusted for each case to obtain a given 2DEG density in the channel. The effects of quantum confinement is modeled through the solution of Schrödinger equation, given by eq. 4, along with...
other fundamental device equations.

\[-\frac{\hbar^2}{2m^*} \frac{d^2 \psi_n(y)}{dy^2} + V(y) \psi_n(y) = E_n \psi_n(y) \tag{1}\]

Where, \(V(y) = -e\phi_e(y) + V_h(y)\) is the effective potential. Here, \(V_h(y)\) is the step potential barrier at the interface, and \(\phi_e(y)\) is the electrostatic potential.

This provides the quantized density of states under the influence of quantum well potential. Here, \(E_n\) and \(\psi_n\) are the \(n^{th}\) bound state energy and wavefunction respectively. A similar set of equations can be used to describe holes.

The discrete nature of the quantized density of states allows to reduce the integral to a sum over bound state energies and the electron density can be given by:

\[N_e = \frac{m^* k_B T}{\pi \hbar^2} \ln \left[ 1 + e^{\left(\frac{E_F - E_n}{k_B T}\right)} \right] \tag{2}\]

This can be, in turn, used as an input to the Poisson equation given by:

\[\frac{d^2 \phi_e(y)}{dy^2} = \frac{e}{\varepsilon_0 \varepsilon_r} \left[ \sum_i N_i \psi_i^*(y) + N_A(y) - N_D(y) \right] \tag{3}\]

Here, \(e\) is the electronic charge, \(\varepsilon_0\) is the permittivity of free space and \(\varepsilon_r\) is the dielectric constant. \(N_i\) is the number of electrons in the \(i^{th}\) subband. \(N_A(y)\) and \(N_D(y)\) are the acceptor and donor concentrations respectively. Also, \(E_F\) is the Fermi energy, \(k_B\) is the Boltzmann constant and \(T\) is the temperature.

The solution to this equation provides potential which can be further substituted into Schrödinger equation for the next iteration. This keeps going until a convergence is achieved and a self-consistent solution of Schrödinger-Poisson equation is found.

The above equations are solved using Silvaco Atlas for the heterostructure used in this work and the eigenvalues and eigenvectors corresponding to the first five subbands are found. The electrons with higher energy (above fifth subband) are no more confined and have finite probability density away from the interface, as shown in fig 3(b), and hence assumed to be bulk like. The inset of fig 3(b) shows a close-up of the wavefunctions near the interface. As we move higher in the bands, the electrons becomes more bulk-like and start moving away from the interface into the bulk as they are no more confined. This reduces the corresponding probability density near the interface which is expected to affect the scattering rates as we will see in the next section. The transverse electric field at the interface is also extracted to calculate interface roughness scattering.

C. Scattering rates

Electrons in the heterostructure devices are subject to scattering from remote impurities, interface roughness, irregularities in the alloy and the phonons. An accurate description of such scattering mechanisms is critical for high field transport study. All the major elastic scattering mechs. such as alloy disorder, remote impurity and interface roughness as well as inelastic scattering mechs. such as polar optical, non-polar optical and acoustic phonon scatterings are taken into account.

Fig 4 shows a schematic of carrier transport under high electric field. The whole system is divided into a 2D and a 3D regime based on a cutoff-energy. Electrons in each region experience drift by the applied electric field and scattering by the perturbed potentials. Unlike the electron transport under low field, the high-field could push the electrons to higher subbands and even to higher conduction bands once the electron has transitioned to the bulk. Hence, we must consider the intersubband scattering processes when the electron is confined and interband scattering processes once it has escaped the confinement. The scattering in the 2DEG is limited by an energy cutoff (0.3 eV), where the 2D-3D transition happens. This energy cutoff is decided based on the confinement potential energy coming from the Schrödinger-Poisson solution. The 2D-3D & 3D-2D transitions are mediated through scattering as well as drift five subbands are taken into account below 0.3 eV in the 2DEG as the higher subbands have very small energy difference with bulk characteristics. Only intra-subband transitions are screened in case of elastic processes as all inter-subband transitions would re-

**TABLE I.** Material parameters used in self-consistent calculation of \(\beta-(\text{Al}_0.2\text{Ga}_{0.8})\text{O}_3/\text{Ga}_2\text{O}_3\) heterostructures. The data is taken from [42-44].

| Parameter               | Value       |
|-------------------------|-------------|
| \(m^*\)                 | 0.3\(m_e\)  |
| Bandgap \(E_g\)         | 4.7 eV      |
| Bandgap \(E_g\)         | 5.0 eV      |
| Band-offset \(\Delta E\) | 0.54 eV     |
| Donor energy \(E_d\)    | 0.135 eV    |
| Dielectric constant \(\varepsilon_r\) | 10          |
quire higher $q$ where the screening factor vanishes. The POP modes are dynamically screened as described later in this section. The non-polar modes are calculated from first principles and each mode is treated separately while calculating the corresponding 2D scattering rates. Here, acoustic modes and non-polar optical phonon modes are treated together and hence we use non-polar to refer them all for convenience. This eliminates any curve fitting and hence the deformation potential constants and also prohibits the use of Thomas-Fermi type screening. To avoid any related errors, the non-polar transitions are kept unscreened. Also, since the non-polar scattering is a high $q$-process, the screening becomes weak and ineffective, justifying our assumption.

For the electrons in the bulk ($>0.3$ eV), the scattering is through POP and non-polar (non-polar optical plus acoustic) modes only as any ionized impurity scattering drops quickly at higher energies and would not contribute much at higher fields. As the 2DEG is confined in a quantum well, limited by a given energy, the average electron density (over the channel region) drops rapidly in the bulk and so the scattering processes in the same are assumed to be free of any screening. The POP EPI elements are then calculated assuming low electron density in the bulk such that the plasmon energy is way below the range of LO phonon energies with no LOPC or dynamic screening present. First 2 conduction bands are considered and the inter-band scattering is assumed to be only mediated by non-polar modes as, due to POP scattering being a small $q$ process, the overlap between the two wavefunctions (orthogonal) vanishes and the corresponding scattering rate becomes negligible.

The scattering rates are calculated based on Fermi’s golden rule as given by:

$$ S(\vec{k}_i, \vec{k}_f) = \frac{2\pi}{\hbar} |H_{k_i,k_f}^e|^2 |I_{m\nu}|^2 \delta(E(\vec{k}_f) - E(\vec{k}_i) - \hbar\omega) + \frac{2\pi}{\hbar} |H_{k_i,k_f}^e|^2 |I_{m\nu}|^2 \delta(E(\vec{k}_f) - E(\vec{k}_i) + \hbar\omega) $$

where,

$$ E_{eff} = \int_{-\infty}^{\infty} \psi_n(y) \frac{dV}{dy} \psi^*_m(y) dy $$

Here $\frac{dV}{dy}$ is the electric field along the confinement direction, which pushes the electrons to collide with the interface.

The alloy disorder momentum relaxation rate is calculated using

$$ \frac{1}{\tau_{Alloy}} = \frac{m^* \Omega_{xc}(1-x) (\delta E_c)^2}{2\pi\hbar^2} F_{al} \int_0^{2\pi} \frac{1 - \cos\theta}{S(q)^2} d\theta $$

The unit cell volume at each Al concentration is taken from interpolating the available data. The scattering potential is assumed to be equal to the conduction band offset $\delta E_c$ between Al$_2$O$_3$ and Ga$_2$O$_3$.

Fig. 3(a-c) show the 2D-2D scattering rates for different elastic scattering mechanisms for the first 5 subbands in the 2DEG at 300 K. The scattering rates shown are unscreened for the purpose of discussion in order to clearly understand the trend but a Thomas-Fermi type screening (only for intra-subband transitions as the inter-subband transitions involve large $q$) is used for the transport calculation. As discussed in the previous section (fig. 2(b)), as we move higher in subbands, the electrons become more delocalized as they move away from the interface and start behaving more like free electrons and hence increasing the probability in the bulk. At the same time, the probability near the interface decreases to keep the overall probability 1. This is being reflected in the

\[
S(\vec{k}_i, \vec{k}_f) = \frac{2\pi}{\hbar} |H_{k_i,k_f}^e|^2 |I_{m\nu}|^2 \delta(E(\vec{k}_f) - E(\vec{k}_i) - \hbar\omega) + \frac{2\pi}{\hbar} |H_{k_i,k_f}^e|^2 |I_{m\nu}|^2 \delta(E(\vec{k}_f) - E(\vec{k}_i) + \hbar\omega)
\]
FIG. 5. The 2D-2D (a) remote, (b) interface roughness, and (c) alloy disorder scattering rates (300 K) as a function of electron energy (eV) for the first 5 subbands. The 0 eV is assumed to be the bottom of the 1st conduction band. The scattering rates shown are unscreened for the purpose of discussion. This heterostructure corresponds to \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \), \( d = 3 \text{ nm} \), 20% Al in the alloy and roughness parameters: \( L = 5 \text{ nm} \), \( \delta = 0.5 \text{ nm} \).

scattering rates in the figure. Since the amount of wavefunction interacting with the impurity decreases near the interface, we see a lowering in the remote impurity scattering rate at higher subbands near the minima. The strong inverse \( q \) dependence weakens the jumps due to density of states. Similarly, the interface roughness gives higher scattering rate initially at higher bands but then drops rapidly due to inverse \( q \) dependence. A large drop at the minima for higher bands is due to effective electric field dependence which is maximum near the interface. Small jumps due to the density of states can be observed when looked carefully. Since, the electrons are more free to leak into the bulk than in the alloy (barrier), the total contribution (leakage) into the alloy decreases as we move higher in bands and hence the alloy disorder scattering rate is smaller for higher bands. Since, alloy disorder is isotropic in nature, we can clearly see jumps due to sudden changes in the density of states.

2. Inelastic scattering rates: Polar optical phonon, Non-polar optical phonon & Acoustic phonon (2D-2D, 2D-3D, 3D-2D & 3D-3D)

As stated before, POP modes limit the low field electron mobility in the bulk of \( \beta \)-Ga\(_2\)O\(_3\) and hence are expected to do the same in heterostructures. However, as already discussed, a very high electron density which can be achieved in the 2DEGs of heterostructures, making the plasmon energy match with the energies of LO phonon modes. The two modes start influencing each other under resonance and form a set of coupled modes called LO phonon-plasmon coupled (LOPC) modes\(^{[53-55]}\). This has been studied in several materials\(^{[27][25]}\) including the bulk of \( \beta \)-Ga\(_2\)O\(_3\)\(^{[336,66,67]}\). At the same time, plasmon oscillating at comparable energy as LO phonons can screen (\( \omega_P > \omega_{LO} \)) the TO-LO splitting or enhances the LO phonon potentials strength through antiscreening (\( \omega_P < \omega_{LO} \))\(^{[55]}\). The dynamic screening in \( \beta \)-Ga\(_2\)O\(_3\) comes from of 12 IR active modes and high energy plasm.

The first order approximation for the 2D plasmons yield:

\[
\omega_P = \sqrt{\frac{\hbar^2 n_{2D} e^2 q}{m^* \epsilon_\infty}}
\]  
(11)

The LOPC modes corresponding to each \( \vec{q} \) is calculated under plasmon-pole approximation given by\(^{[66,68]}\):

\[
\epsilon_\infty(\vec{q}) = \epsilon_\infty \prod_{i=1}^{12} \left( \frac{(\omega_{LO}^i(\vec{q}))^2 - \omega^2}{(\omega_{TO}^i(\vec{q}))^2 - \omega^2} - \frac{\epsilon_\infty \omega_P^2}{\omega^2} \right)
\]  
(12)

The scattering is still through LO modes as plasmons would only offer momentum exchange between the electrons rather than providing any average momentum relaxation for the ensemble. This means we must find the LO mode contribution to each LOPC modes.

The modified Fröhlich vertex gives the scattering strength for the electron-phonon interaction\(^{[66,68]}\):

\[
\left| M_{LO}^{\nu,LO}(\vec{q}) \right|^2 = \frac{e^2}{2\Omega_0} \left[ \frac{\omega_{LO}^{\nu,LO}(\vec{q})}{q^2} \left( \frac{1}{\epsilon_{\omega_\nu}^{\nu,LO}(\vec{q})} - \frac{1}{\epsilon_{\omega_\nu}^{\nu,LO}(\vec{q})} \right) \Lambda_{\nu}^{LO}(\vec{q}) \right]
\]  
(13)

A pair of dielectric constants \( \epsilon_{\omega_\nu}^{\nu,LO}(\vec{q}) \) and \( \epsilon_{\omega_\nu}^{-LO}(\vec{q}) \) must be calculated for each LO mode corresponding to a given LOPC mode. Here, \( \epsilon_{\omega_\nu}^{\nu,LO}(\vec{q}) \) includes the full response of that LO mode, while \( \epsilon_{\omega_\nu}^{-LO}(\vec{q}) \) includes the response of all
other modes keeping that LO mode frozen.

At very high electron density, plasmons cease to behave as a collective excitation in the electron-hole pair continuum (EHC) and would affect the coupling. This is taken into account by taking off the plasmon dispersion from the calculation according to the upper boundary of EHC, given by

$$\omega_k(q) = \frac{\hbar^2 k_F q}{m^*} + \frac{\hbar^2 q^2}{2m^*}, \quad k_F$$

is the Fermi vector at zero temperature.

The scattering rate gets impacted by screening as well as the anti-screening of POP phonons through the 2D plasmons. Fig. 6 shows the LOPC modes calculated for $n_{2D}$=5×10^{12} cm^{-2} in cartesian x direction. There are 9 LOPC corresponding to 8 LO modes polarized in x-z plane ($B_\alpha$). For very low electron density, when the plasmon energy is way below the range of POP energies, there is no screening involved and the corresponding scattering strength is unscreened. When the electron density is such that the corresponding plasmon energy is in the range of POP energies, the POP modes with lower energy get screened and the ones with higher energy get anti-screened. As the 2D plasmon energy is also proportional to the magnitude of the wavevector $q$ to the first order of approximation, the number of modes getting screened increases with $q$. However, due to long range nature of such phonons, the scattering strength decreases and hence at low 2DEG densities, the anti-screening dominates and limits the overall low field mobility. However, at very high electron densities, the rate of increase in 2D plasmon energy is higher (higher slope) and hence even at smaller $q$, multiple modes get screened.

Fig. 6 shows the LOPC frequencies calculated for $n_{2D}$=5×10^{12} cm^{-2} corresponding to 8 LO modes polarized in x-z plane ($B_\alpha$). The black dotted line represents the first order variation of plasmon frequency.

The escape and capture of electrons from and into the 2DEG is another important transition which must be considered. The 2D-3D and 3D-2D transitions happen though phonon absorption and emission respectively. This is usually ignored in simple Monte Carlo models for the 2DEG where such transitions are mediated only through drift. The scattering rate calculation follows the same process as 2D scattering with some modifications. The overlap integral is now between a confined wavefunction and a 3D wavefunction (more like a free electron). The 3D wavefunction for a given $k$ is calculated through Gram-Schmidt method such that it is orthogonal to each subband wavefunction. For 2D-3D scattering, the final state ranges from 0.3-0.5 eV (limited by maximum phonon energy) and is in the 3D k-space. For 3D-2D scattering, the initial 3D-wavevector again only ranges from 0.3-0.5 eV and the final state could lie in any of the subbands. The overlap integral takes care of the momentum conservation. Fig. 7(c) shows the polar optical and non-polar phonon scattering rates (below 0.3 eV) for the first 2 conduction bands in bulk. The 3D scattering rates are only calculated until 3 eV following a previous Monte Carlo report for the bulk where the electron distribution drops to zero beyond 3 eV above electric field considered in this work. Note that the electrons near 0.3 eV can emit and jump to lower energies but that kind of transition is considered under 3D-2D scattering as discussed later. An increasing non-polar scattering rate with energy shapes the velocity-field curve at higher fields. The anisotropy in the scattering rates, coming from the anisotropy in the phonons, is clearly visible and is expected to impact our Monte Carlo calculations.

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FIG. 7. The 2D-2D (a) polar optical phonon (POP), and (b) non-polar (non-polar optical plus acoustic) phonon scattering rates (300 K) as a function of electron energy (eV) for the first 5 subbands. Anisotropy is clearly visible from the scattered points. The 0 eV is assumed to be the bottom of the 1st conduction band. This heterostructure corresponds to \( n_{2D} = 5 \times 10^{12} \) cm\(^{-2}\), \( d = 3 \) nm, 20% Al in the alloy and roughness parameters: \( L = 5 \) nm, \( \delta = 0.5 \) nm. (c) The 3D-3D polar optical phonon (Polar), and non-polar (non-polar optical plus acoustic) phonon scattering rates (300 K) as a function of electron energy (eV) for the first 2 conduction bands (denoted in brackets). Anisotropy is clearly visible from the scattered points. The 0 eV is assumed to be the bottom of the 1st conduction band.

FIG. 8. The (a) 2D-3D (300 K, only absorption) & (b) 3D-2D (300 K, only emission) polar optical phonon (POP), and (c) 2D-3D (300 K, only absorption) & (d) 3D-2D (300 K, only emission) non-polar (non-polar optical plus acoustic) phonon scattering rates as a function of electron energy (eV). Anisotropy is clearly visible from the scattered points. The 0 eV is assumed to be the bottom of the 1st conduction band. This heterostructure corresponds to \( n_{2D} = 5 \times 10^{12} \) cm\(^{-2}\), \( d = 3 \) nm, 20% Al in the alloy and roughness parameters: \( L = 5 \) nm, \( \delta = 0.5 \) nm.
III. FULL-BAND MONTE CARLO

The full-band Monte Carlo (FBMC) approach\textsuperscript{72–77} is the most comprehensive and accurate method to solve the Boltzmann transport equation (BTE), governing the electron dynamics in the semi-classical regime. This method is an extension of general random sampling technique used to solve any multi-dimensional integral problem. For transport problems, a random walk is performed by the charge carriers to simulate their stochastic motion under the influence of several scattering processes.

The idea is to simulate the carriers moving as free particles, subject to instantaneous random collisions. This is done through randomly generating free-flight times following\textsuperscript{75}

\[ t_0 = \frac{-1}{\Lambda} \ln(r), \]

where \( r \) is a random number and \( \Lambda \) is the maximum total scattering rate at any \( k \) in a given subband/band. The random numbers, for a given core during a parallel computation, are computed by initially providing a random seed to avoid any duplication. The free particle motion is governed by\textsuperscript{75}

\[ k_{\text{new}} = k_{\text{old}} - \frac{\vec{E}t}{\hbar}, \]

where \( k \) is the crystal momentum and \( \vec{E} \) is the applied electric field in a given direction. If an electron in the 2DEG ends up at a higher energy than the cutoff during a drift process, a random number is used to select a given state such that the in-plane momentum and the total energy (\( E_{\text{tot}} \)) is conserved. Similarly, when an electron in the bulk loses energy during the drift process, the final subband \( n \) is chosen such that the in-plane momentum is conserved and the total energy follows: \( E_n < E_{\text{tot}} < E_{n+1} \). If the energy falls below that of the first subband, the electron is placed in the first subband. This, however, violates the energy conservation rule which is an assumption here. The drift process is followed by randomly choosing a scattering event through rejection technique and finally finding the final state with new momentum and energy. This is then repeated until a convergence in an observable is achieved. An ensemble of particles are simulated to study the time-dependent evolution of physically observable quantities such as average drift velocity, average energy, etc. These quantities are calculated at different sampled times where the motion of each particle is synchronized.

An ab-initio based FBMC simulator is developed from scratch, to investigate the high field transport in the 2DEG of heterostructures. The program is basically designed to perform three critical functions as discussed next:

A. Initial distribution

The first step in the process is to initialize the particles based on Fermi-Dirac distribution. This approaches to Maxwell-Boltzmann distribution at high temperature and for non-degenerate doping. The Fermi-level is first calculated through ab-initio calculated density of states at a given temperature and electron density. A given number of particles are then distributed randomly such that they follow the same distribution. The wavevector \( \vec{k} \) corresponding to a given energy is then computed through a process similar to final state selection (explained later). Note that the electrons are assumed to occupy only the first subband when no field is applied in all cases. Fig. 9 shows the distribution of 5000 electrons for \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \), and \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \). The electrons are assumed to occupy only the first subband at zero electric field. The 0 eV is assumed to be the bottom of the first subband. Since the same number of electrons are simulated in both the cases, the electrons from the lower energy have moved to fill the higher energy states in the latter as the Fermi level moves up in the 1st subband.

FIG. 9. The initial distribution of 5000 electrons based on a Fermi-Dirac distribution function at 300 K for (a) \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \) and (b) \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \). The electrons are assumed to occupy only the first subband at zero electric field. The 0 eV is assumed to be the bottom of the first subband. Since the same number of electrons are simulated in both the cases, the electrons from the lower energy have moved to fill the higher energy states in the latter as the Fermi level moves up in the 1st subband.
B. Normalized scattering rates

The next step is to select a scattering process from all mechanisms which would instantaneously scatter the particle and provide a new final state. The 2D and 3D scattering rates are calculated and stored for each \( k \), initial and final subband/band and mode, type of mechanism (absorption/emission) in case of phonon involving scattering. The scattering rates corresponding to each mechanism are efficiently stored in a multidimensional array for each \( k \) and subband/band and a separate tag keeps the information of the final state, mode and type of mechanism involved. Whenever a scattering mechanism has to be selected, a hashing method is used to quickly pickup all the scattering rates for a given \( k \) and subband/band along with the tags. A given scattering is normalized as \(^{73}\)

\[
S_{\text{nrm}}^n(m\vec{k}) = \frac{\sum_{i=1}^n S_i(m\vec{k})}{\Lambda} \tag{14}
\]

Where, \( n \) is the \( n \)th mechanism, \( m \) is the band/subband and \( \Lambda \) is the sum of all possible scattering mechanisms at \( m\vec{k} \). A given scattering mechanism is then stochastically selected using a random number such that \( S_{\text{nrm}}^n(m\vec{k}) > r > S_{\text{nrm}}^{n-1}(m\vec{k}) \). The electron is considered to be self-scattered if \( r > S_{\text{nrm}}^n(m\vec{k}) \), where \( p \) is the total number of scattering mechanisms, and the final state remains the same.

The memory requirement is huge and increases with \( N_k \times N_p \times N_m \) due to dense k-points, multiple bands and modes respectively but a heavy RAM for each core in a given node is utilized to cope with the same.

C. Final state selection

The most computationally intensive step in the FBMC program is finding the final state of an electron once a scattering event has occurred. Since, this involves many small subprocesses in order to accurately find the final state, the overall process is relatively slow and determines the total computation time of the FBMC program. Here, we discuss the elastic and inelastic scattering cases separately.

1. Elastic scattering

The elastic scattering rate tag includes the information on final subband and hence the final state is searched through that particular band such that the momentum and energy is conserved. For isotropic scatterings, the angle between the initial and the final states is simply given by \( \phi=2\pi r \), where, \( r \) is a random number in \((0,1)\) \(^{23}\). For anisotropic scatterings, for a given \( k \), the scattering rate is first calculated for a given set of discrete \( q \) (determined by \( \theta \)) on a dense mesh and is then normalized by the total scattering rate as discussed before. A final state \((\theta)\) is selected such that \( S_{\text{nrm}}^n(m\vec{k}) > r > S_{\text{nrm}}^{n-1}(m\vec{k}) \), where \( r \) is a random number in \((0,1)\). This automatically takes into account the anisotropic nature of the scattering mechanism as each possible final states are weighted with the corresponding matrix element. The final state \((k_f,k_f)\) is then calculated by running an in-plane momentum conservation and total energy conservation on a fine grid. This final state is again limited by the density of chosen mesh. The next step would be to chose a random state within the square spanned (for a 2D k-space) by a given \( k \) point. This is explained later in this section.

2. Inelastic scattering

Here, we explain the final state selection for a 3D region\(^{25}\) and a similar set of steps would apply in 2D but on a 2D k-space. First, all the k-points satisfying the energy and momentum conservation corresponding to a given mode \((\nu)\) and mechanism (absorption/emission-) within a certain smearing factor \((E_{mk} - E_{nk} \pm \hbar \nu \omega_{\nu} \leq 0.01eV)\) are shortlisted. This is an intense process and requires heavy computing resources. A full phonon dispersion on a dense grid increases the complexity. An improvement can be achieved by hashing the band structure and phonon dispersion for an easy access. This gives all the \( q \)-points that would satisfy the energy-momentum conservation for a given mode \((\nu)\). The next step is to find the matrix elements (EPI elements) \( g(k_i,k_j - k_i)^{\nu} \) corresponding to the shortlisted \( q \) points. This is done, as explained earlier, by storing the matrix elements which satisfy the energy-momentum conservation relation on an already defined grid. This significantly reduces the storage issue. Such matrix elements are stored in multiple files out of which a given file is first selected based on k-q hashing and then only the corresponding (to shortlisted points) file is read. Now, a final state \((k_f)\) is picked stochastically, using a random number, based on the product of \(|g(k_i,k_j - k_i)|^2\) and local density of states (LDOS)\(^{28}\). Here, the LDOS is proportional to the area contributed by an equienergy surface \((E_{mk} \pm \hbar \nu \omega_{\nu})\) to a given cube (spanned by a k-point). This is shown in fig 10(a). Once a cube is picked, the final state would lie inside that cube on that equienergy surface. Now, the shape of surface cut by the equienergy surface is determined followed by dividing it into smaller triangles. There are multiple shapes possible and hence the number of triangles could be more than 2. Now, a given triangle is selected stochastically using a random number. Once, we have a triangle as shown in fig.22(a), the final state is given by\(^{29}\)

\[
k_f = \vec{a} + \lambda_1 (\vec{b} - \vec{a}) + \lambda_2 (\vec{c} - \vec{a}) \tag{15}
\]

Where, \( \lambda_1 = 1 - \sqrt{1-r}, \lambda_2 = r(1-\lambda_1) \) and \( r \) is a random number in \((0,1)\).

The final state lies on a 2D k-space for the electrons in the 2DEG as shown in fig 10(b). An equienergy line would cut the square spanned by a given k-point where the length of the line inside the square would correspond to the contributed LDOS. After selecting a single square, the final state is simply given by\(^{29}\)

\[
k_f = \vec{a} + \lambda_1 (\vec{b} - \vec{a}) \tag{16}
\]

When the electron is at higher energy and non-polar scattering rates become significant, the program starts accessing the matrix element files and the RAM requirement shoots up. This
again increases the complexity of this step and the overall pro-
gram run time. Several independent processes using sufficient
RAM are run using mpi4py to better handle this issue.

IV. RESULTS AND DISCUSSION

The Monte Carlo simulation is performed with an ensem-
ble of 5000 electrons for a certain number of cases involving
different 2DEG densities and also an experimental structure
for comparison and the corresponding results are presented
here. We discuss the evolution of electron population and their
transient dynamics with electric field for a given heterostruc-
ture with \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \) and \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \) respectively at 300 K. The electric field value ranges from 10
kVcm\(^{-1}\) to 400 kVcm\(^{-1}\) applied in cartesian \(-x\) direction. The
two cases are compared to provide an insight on the effect
of LOPC screening on POP scattering and hence on the be-
haviour of electron transport in the 2DEG. The heterostructure
under consideration corresponds to \( d = 3 \text{ nm}, 20\% \text{ Al in the}
alloy and roughness parameters: } L = 5 \text{ nm}, \delta = 0.5 \text{ nm}. How-
ever, the velocity field curves are discussed for a few more
cases to provide a fair comparison between our calculation
and the available experimental data.

A. Zone population

Under high field, the electrons have distribution covering
the whole brillouin zone. Fig. 11(a-f) show the evolution of
an ensemble of electrons with energy at electric fields: 10
kVcm\(^{-1}\), 150 kVcm\(^{-1}\) and 300 kVcm\(^{-1}\) for electron densi-
ties: \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \) and \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \) respec-
tively. The initial distribution function follows Fermi-Dirac
at zero field as discussed before. The distribution is collected
once the steady state has reached at a given applied electric
field. The distribution dies off quickly after \( \sim 2 \text{ eV} \) in both
the cases even at 300 kVcm\(^{-1}\). The velocity saturation re-
sults from the short range intra-valley EPI. The satellite val-
ley, as discussed before, lies around \( \sim 2.5 \text{ eV} \) and hence the in-
tervalley scattering is not responsible for negative differential
conductance (NDC). The non-parabolicity of the conduction
band at higher energies reduces the average electronic veloci-
ties and results in the NDC unlike the mechanism observed in
the bulk of GaAs and GaN (due to intervalley scattering).

The antiscreening offered by LOPC phonon in the former
case \( (n_{2D} = 1 \times 10^{12} \text{ cm}^{-2}) \) at higher energies, as discussed be-
fore, causes high 2D-2D scattering in the 2DEG and hence de-
creases the drift rate. Comparatively, the screening dominates
when \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \) and hence the drift rate is larger
shaping the distribution function accordingly. A kink near 0.3
\text{ eV}, as seen in both the cases, is due to low 3D-2D scattering
rate causing it difficult for the electrons to get captured back
into the 2DEG.

The distribution in k-space once the steady state has

![FIG. 10. (a) The equienergy surfaces cutting a cube spanned by a k-point in the 3-D reciprocal space, with the contribution weight denoted
by the shaded greenish region. (b) The equienergy line cutting a square spanned by a k-point in the 2-D reciprocal space, with the contribution
weight denoted by the green line (between a-b). This is an important step in stochastically determining the final state which can be anywhere
on the surface/line.](image-url)
FIG. 11. (a-c) & (d-f) show the steady state electron population with energy (eV) at electric field of 10, 150 and 300 kVcm\(^{-1}\) (in -x direction) for (a-c) \(n_{2D} = 1 \times 10^{12} \text{ cm}^{-2}\), and (d-f) \(n_{2D} = 5 \times 10^{12} \text{ cm}^{-2}\) respectively. The screening in the latter case causes more number of electrons to occupy the higher energy states at higher fields. A kink at the 2D-3D boundary is a result of low 3D-2D scattering rate making it difficult for the electrons to bounce back into the 2DEG.

FIG. 12. (a-c) show the evolution of electron population (steady state) in all the 5 subbands (colored) and in the bulk (gray) in a 2D k-space for \(n_{2D} = 1 \times 10^{12} \text{ cm}^{-2}\) at electric field of (a) 10, (b) 150 and (c) 300 kVcm\(^{-1}\) (in -x direction). (d-f) show the evolution of electron population (steady state) in all the 5 subbands (colored) and in the bulk (gray) in a 2D k-space for \(n_{2D} = 5 \times 10^{12} \text{ cm}^{-2}\) at electric field of (d) 10, (e) 150 and (f) 300 kVcm\(^{-1}\) (in -x direction). Note that electrons in the bulk have all three momentum components but the \(k_y\) is omitted in the figure for presentation. The overall shift in +x direction due to field (in -x) can be clearly seen. Also, the population in the 2DEG (colored dots correspond to different subbands: see legend) is seen to be decreasing with the field as electrons become more bulk type.
reached is shown in fig[12]a-c)&(d-f) when the field is applied in -x direction for \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \) and \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \) respectively. The colored dots correspond to the electrons in the 2DEG (x-z component) whereas the gray dots are the 3-D electrons with y momentum component omitted for a better presentation. An almost symmetric distribution at 10 kVcm\(^{-1}\) shifts to x region when higher field is applied. A significant population in the -x direction is due to high non-polar momentum relaxation rate as compared to low energy relaxation. The net current is due to the contribution from the overall distribution. Another interesting thing to notice here is shift in the electron population from the 2DEG subbands to the bulk with applied electric field. The shown region only covers 40% of the entire brillouin zone and hence it can be inferred that the zone edges are not populated with enough electrons due to the high non-polar scattering rates.

B. Transient dynamics

The transient dynamics in Monte Carlo simulation becomes very important when studying a scaled device where the channel length is short enough for the electrons to not reach the steady state while drifting from source to the drain terminal. For applications in high power electronics, this won’t play a significant role. However, as we have thoroughly discussed before that \( \beta - \text{Ga}_2\text{O}_3 \) finds its application in RF switching as well, where the scaling of the devices matters, hence making it critical to discuss such characteristics here.

The velocity-time plot for \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \) and \( n_{2D} = 5 \times 10^{12} \text{ cm}^{-2} \) at different electric field values (10,50,100,150,200,250,300,350,400) kVcm\(^{-1}\) is shown in fig[13]a)&(b) respectively. An ensemble of 5000 electrons is simulated and the velocity of each of them is extracted and then averaged out when their motion is synchronized (at a given time). At lower electric fields, the POP scattering is dominant and hence a smooth transition to a steady state can be seen in the velocity. This is due to low momentum and energy relaxation provided by polar optical phonons. At higher fields, when the electrons are in the bulk, the non-polar scattering starts kicking in and rapidly increases the momentum relaxation rate while keeping the energy relaxation still limited by the available phonon energies. This causes the velocity to shoot up due to lower momentum randomization (limited by POP) and then drop down to attain a steady state due to higher momentum randomization (limited by non-polar phonons). On the other hand, there is a smooth change in the energy until the steady has reached. The velocity overshoot in the former case (a) is not seen until a high field (300 kVcm\(^{-1}\)) is applied. This is due to high POP scattering rate (antiscreening from LOPC) in the 2DEG. However, the more screening in the latter case (b) enables the electrons to enter into the bulk at even lower field (150 kVcm\(^{-1}\)) and get impacted by the non-polar scattering, causing an early velocity overshoot. A device length defined by the area under the overshoot curve can take advantage of the high velocity for RF switching applications. This, however, would require higher 2DEG density and smaller device length for the screening to dominate and provide higher velocity as seen in the figure.

C. Velocity-field curves

Fig[14] shows a comparison between velocity-field curves for a few heterostructures and the bulk \( \beta - \text{Ga}_2\text{O}_3 \). This is an important topic of discussion as the characteristics curves of a device depend on the impact of high field on the velocity of carriers. The experimental heterostructure is similar to the one used in this work with spacer thickness changed to \( d = 4.5 \text{ nm} \) to give an electron density of \( n_{2D} = 1.8 \times 10^{12} \text{ cm}^{-2} \) in the 2DEG[22]. Before further discussion, it’s important to reiterate here that the velocity saturation is resulting from in-travalley non-polar scattering in the bulk region and the NDC seen is simply a reflection of non-parabolicity of the \( \Gamma \) valley at higher energies. The net velocity is the contribution from all the electrons and hence is a strong function of distribution.
in the momentum-energy space.

As seen in fig. 14(a), the peak corresponding to \( n_{2D} = 5 \times 10^{12} \) (calc.) lies at around the same field (250 kV cm\(^{-1}\)) as bulk but with higher velocity (\( \sim 2.25 \times 10^6 \) cm\(^{-1}\)). This is due to screening present in the 2DEG reducing the corresponding population at lower energies. The corresponding low field (10 kV cm\(^{-1}\)) mobility is (\( \sim 393 \) cm\(^2\)V\(^{-1}\)s\(^{-1}\)). The velocity at the same field is low for \( n_{2D} = 1 \times 10^{12} \) (calc.) at 300 K and peaks at 350 kV cm\(^{-1}\). This is due to the electron population in the 2DEG (low energies) even at 250 kV cm\(^{-1}\) as seen before (due to higher POP scattering) making the overall velocity low. The peak velocity is comparable to bulk for \( n_{2D} = 1 \times 10^{12} \) and slightly higher for \( n_{2D} = 1.8 \times 10^{12} \) due to their respective low field (10 kV cm\(^{-1}\)) mobility values of (\( \sim 107 \) cm\(^2\)V\(^{-1}\)s\(^{-1}\)) and (\( \sim 190 \) cm\(^2\)V\(^{-1}\)s\(^{-1}\)) respectively.

The low field (10 kV cm\(^{-1}\)) mobility corresponding to the calculated experimental structure at 50 K is \( \sim 1220 \) cm\(^2\)V\(^{-1}\)s\(^{-1}\), and the velocity peaks at 250 kV cm\(^{-1}\) around (\( \sim 2.5 \times 10^6 \) cm\(^{-1}\)) coming from higher low field mobility. This is shown in fig. 2(b). The discrepancy between the two could be attributed to the contact resistance contribution in the measured values which would compress the overall plot along the field axis. The other possible reason could be the self-heating effect [ref], which is ignored in this work and is supposed to decrease the net velocity at higher fields. The error bars correspond to 10\% variation in the electron effective mass.

V. CONCLUSION

The high field electron transport in the 2DEG of \( \beta-(\text{Al}_2\text{Ga}_{1-x})\text{O}_3/\text{Ga}_2\text{O}_3 \) heterostructures is investigated using full-band Monte Carlo approach. An in-house developed program is utilized to extract the parameters under interest such as velocity field curves, velocity-time plots etc which can ultimately be used to design improved devices for better performance. A comparison between a few heterostructure devices and the bulk is presented with the maximum velocity reaching up to \( \sim 2.25 \times 10^6 \) cm\(^{-1}\) at 300 K for \( n_{2D} = 5 \times 10^{12} \) with the electric field value of 250 kV cm\(^{-1}\) comparable to bulk.

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DATA AVAILABILITY STATEMENT

The data and the in-house developed programs that support the findings of this study are available from the corresponding author upon reasonable request. The ab-initio calculations are performed using the open source software, Quantum Espresso. The licensed version of Silvaco Atlas is used for the self-consistent Schoringer-Poisson calculations.

1. M. N. Hasan, E. Swinnich, and J.-H. Seo, “Recent progress in gallium oxide and diamond based high power and high-frequency electronics,” Wide Bandgap Semiconductor Electronics and Devices, 63–78 (2020).
2. M. Higashiwaki and G. H. Jessen, “Guest editorial: The dawn of gallium oxide microelectronics,” (2018).
3. M. N. Hasan, E. Swinnich, and J.-H. Seo, “Recent progress in gallium oxide and diamond based high power and high-frequency electronics,” Wide Bandgap Semiconductor Electronics and Devices, 63–78 (2020).
4. Z. Liu, P.-G. Li, Y.-S. Zhi, X.-L. Wang, X.-L. Chu, and W.-H. Tang, “Review of gallium oxide based field-effect transistors and schottky barrier diodes,” Chinese Physics B 28, 017105 (2019).
5. X. Yan, I. S. Esqueda, J. Ma, J. Tice, and H. Wang, “High breakdown electric field in \( \beta-\text{Ga}_2\text{O}_3 \)/graphene vertical barristor heterostructure,” Applied Physics Letters 112, 032101 (2018).
1. J. Bae, H. W. Kim, I. H. Kang, G. Yang, and J. Kim, “High breakdown volt-
age quasi-two-dimensional $\beta$-Ga$_2$O$_3$ field-effect transistors with a boron nitrile field plate,” Applied Physics Letters 112, 122102 (2018).

2. Y. Lv, X. Zhou, S. Long, Y. Wang, X. Song, X. Zhou, G. Xu, S. Liang, Z. Feng, S. Cai, et al., “Enhancement-mode $\beta$-Ga$_2$O$_3$ metal-oxide-
semiconductor field-effect transistor with high breakdown voltage over 3000, v realized by oxygen annealing,” physica status solidi (RRL)-Rapid Research Letters 14, 1900586 (2020).

3. K. Zeng, A. Vaidya, and U. Singisetti, “A field-plated ga2o3 mosfet with near 2-kv breakdown voltage and 520 m$\Omega$-cm2 on-resistance,” Applied Physics Express 12, 081103 (2019).

4. J. K. Mun, K. Cho, W. Chang, H.-W. Jung, and J. Do, “2.32 kv breakdown voltage lateral $\beta$-Ga$_2$O$_3$ mosfets with source-connected field plate,” ECS Journal of Solid State Science and Technology 8, Q3079 (2019).

5. S. Sharma, K. Zeng, S. Saha, and U. Singisetti, “Field-lateral $\beta$-Ga$_2$O$_3$ mosfets with polymer passivation and 8.03 kv breakdown voltage,” IEEE Electron Device Letters 41, 836–839 (2020).

6. N. Yadava and R. Chauhan, “recent advances in designing gallium oxide mosfet for rf application,” ECS Journal of Solid State Science and Technology 9, 065010 (2020).

7. K. Chakab, D. Walker, A. Green, A. Crespo, M. Lindquist, K. Leedy, S. Tet-
lak, R. Gilbert, N. Moser, and G. Jessen, “Sub-micron gallium oxide radio frequency field-effect transistors,” in 2018 IEEE MTT-S International Microwa-
ve Workshop Series on Advanced Materials and Processes for RF and THz Applications (IMWS-AMP) (IEEE), 2018, pp. 1–3.

8. N. Moser, K. Liddy, A. Islam, N. Miller, K. Leedy, T. Asel, S. Mou, A. Green, and K. Chakab, “Toward high voltage radio frequency devices in $\beta$-Ga$_2$O$_3$,” Applied Physics Letters 117, 242101 (2020).

9. T. Kamimura, Y. Nakata, and M. Higashiwaki, “Delay-time analysis in radio-frequency $\beta$-Ga$_2$O$_3$ field effect transistors,” Applied Physics Letters 117, 235301 (2020).

10. H. Peelaers and C. G. Van de Walle, “Sub-band-gap absorption in $\beta$-Ga$_2$O$_3$,” Applied Physics Letters 111, 182104 (2017).

11. H. Peelaers and C. G. Van de Walle, “Brillouin zone and band structure of $\beta$-Ga$_2$O$_3$,” physica status solidi (b) 252, 828–832 (2015).

12. H. Gao, S. Muralidharan, N. Pronin, M. R. Karim, S. M. White, T. Asel, G. Foster, S. Krishnamoorthy, S. Rajan, L. R. Cao, et al., “Optical signatures of deep level defects in Ga$_2$O$_3$,” Applied Physics Letters 112, 242102 (2018).

13. S. Oh, M. A. Mastro, M. J. Tadjer, and J. Kim, “Solar-blind metal-
semiconductor-metal photodetectors based on an exfoliated $\beta$-Ga$_2$O$_3$ mi-
cro-flake,” ECS Journal of Solid State Science and Technology 6, Q79 (2017).

14. K. Ghosh and U. Singisetti, “Impact ionization in $\beta$-Ga$_2$O$_3,” Applied Physics Letters 124, 085707 (2018). https://doi.org/10.1063/1.5034120

15. K. Ghosh and U. Singisetti, “Ab initio calculation of electron–photon coupling in monolinic $\beta$–ga$_2$o$_3$ crystal,” Applied Physics Letters 109, 027102 (2016). https://doi.org/10.1063/1.4961308

16. Y. Kang, K. Krishnamwary, H. Peelaers, and C. G. Van de Walle, “Fundamental limits on the electron mobility of $\beta$-Ga$_2$O$_3$,” Journal of Physics: Condensed Matter 29, 234001 (2017).

17. T. Onuma, S. Saito, K. Sasaki, K. Goto, T. Masui, T. Yamaguchi, T. Honda, A. Kuramata, and M. Higashiwaki, “Temperature-dependent excitation reso-
nance energies and their correlation with ir-active optical phonon modes in $\beta$-Ga$_2$O$_3$ single crystals,” Applied Physics Letters 108, 101904 (2016).

18. K. Mengle and E. Kioiak, “Vibrational and electron-photon coupling properties of $\beta$-Ga$_2$O$_3$ from first-principles calculations: Impact on the mo-
delization and breakdown field,” AIP Advances 9, 015135 (2019).

19. A. Parisini, K. Ghosh, U. Singisetti, and R. Fornari, “Assessment of phonon scattering-related mobility in $\beta$-Ga$_2$O$_3$,” Semiconductors and Science and Technol-
ology 33, 105008 (2018).

20. A. Kumar, K. Ghosh, and U. Singisetti, “Low field transport calculation of 2-dimensional electron gas in $\beta$-al$_{1-x}$ga$_x$o$_3$–Ga$_2$O$_3$ heterostructures,” Journal of Applied Physics 128, 105703 (2020). https://doi.org/10.1063/5.0008578

21. Y. W. Zhang, A. Neal, Z. B. Xu, C. Cojishi, J. M. Johnson, Y. H. Zheng, S. Bajaj, M. Brenner, D. Dorsey, K. Chakab, G. Jessen, J. Hwang, S. Mou, J. P. Heras, and S. Rajan, “Demonstration of high mobili-
ty and quantum transport in modulation-doped $\beta$-(Al$_{x}$Ga$_{1-x}$)$_2$O$_3$–Ga$_2$O$_3$ heterostructures,” Applied Physics Letters 112 (2018), Artn 173502.
tature quantum well laser structures,” Applied physics letters 63, 1874–1876 (1993).

46C.-Y. Tsai, L. F. Eastman, Y.-H. Lo, and C.-Y. Tsai, “Carrier capture and escape in multisubband quantum well lasers,” IEEE photonics technology letters 6, 1088–1090 (1994).

47K. Muraki, A. Fujiwara, S. Fukatsu, Y. Shiraki, and Y. Takahashi, “Evidence for resonant electron capture and charge buildup in GaAs/AlGaAs quantum wells,” Physical Review B 53, 15477 (1996).

48M. Lundstrom, Fundamentals of Carrier Transport, 2nd ed. (Cambridge University Press, 2000).

49B. K. Ridley, “The electron-phonon interaction in quasi-two-dimensional semiconductor quantum-well structures,” Journal of Physics C: Solid State Physics 15, 5899–5917 (1982).

50K. Hirakawa and H. Sakaki, “Mobility of the two-dimensional electron-gas at selectivity doped n-type AlGaAs/GaAs heterojunctions with controlled electron concentrations,” Physical Review B 33, 8291–8303 (1986).

51S. Yamakawa, H. Ueno, K. Taniguchi, C. Hamaguchi, K. Miyatsuji, K. Masaki, and U. Ravaioli, “Study of interface roughness dependence of electron mobility in silicon inversion layers using the monte carlo method,” Journal of Applied Physics 79, 911–916 (1996).

52T. Unuma, M. Yoshita, T. Noda, H. Sakaki, and H. Akiyama, “Intersubband absorption linewidth in GaAs quantum wells due to scattering by interface roughness, phonons, alloy disorder, and impurities,” Journal of Applied Physics 93, 1586–1597 (2003).

53B. B. Varga, “Coupling of plasmons to polar phonons in degenerate semiconductors,” Phys. Rev. 137, A1896–A1902 (1965).

54K. S. Singwi and M. P. Tosi, “Interaction of plasmons and optical phonons in degenerate semiconductors,” Phys. Rev. 147, 658–662 (1966).

55B. Ridley, Quantum Processes in Semiconductors (OUP Oxford, 2013).

56C. G. Olson and D. W. Lynch, “Longitudinal optical-phonon-plasmon coupling in GaAs,” Phys. Rev. 177, 1231–1234 (1969).

57R. Cusco, N. Domènech-Amador, F. Hung, W.-Y. Loh, R. Droopad, and L. Artús, “Raman scattering study of lo phonon-plasmon coupled modes in p-type InGaAs,” Journal of Alloys and Compounds 634, 87–93 (2015).

58P. Kozawa, T. Kachi, H. Kano, Y. Taga, M. Hashimoto, N. Koida, and K. Manabe, “Raman scattering from lo phonon-plasmon coupled modes in gallium nitride,” Journal of Applied Physics 75, 1098–1110 (1994) https://doi.org/10.1063/1.356492.

59A. Miyahara, R. Carles, E. Bedel, and A. Muñoz-Yagüe, “Polar phonon-intersubband plasmon coupling in Si delta-doped GaAs,” Journal of Applied Physics 74, 1072–1078 (1993) https://doi.org/10.1063/1.354954.

60L. Artús, R. Cusco, J. Ibáñez, N. Blanco, and G. González-Díaz, “Raman scattering by lo phonon-plasmon coupled modes in n-type InP,” Phys. Rev. B 60, 5456–5463 (1999).

61R. J. Bell, T. J. McMahon, and D. G. Rathbun, “Longitudinal optical phonon-plasmon coupling in cds,” Journal of Applied Physics 39, 48–51 (1968) https://doi.org/10.1063/1.1655776.

62M. V. Klein, B. N. Ganguly, and P. J. Colwell, “Theoretical and experimental study of raman scattering from coupled lo phonon-plasmon modes in silicon carbide,” Phys. Rev. B 6, 2380–2388 (1972).

63L. Farvacque and F. Carosella, “Intrinsic free carrier mobility of quantum wells in polar materials,” Phys. Rev. B 72, 125344 (2005).

64A. Hauber and S. Fahy, “Scattering of carriers by coupled plasmon-phonon modes in bulk polar semiconductors and polar semiconductor heterostructures,” Phys. Rev. B 95, 045210 (2017).

65K. Ghosh and U. Singisetty, “Electron mobility in monolines β – Ga2O3—effect of plasmon-phonon coupling, anisotropy, and confinement,” Journal of Materials Research 32, 4142–4152 (2017).

66M. Schubert, A. Mock, R. Korlacki, S. Knight, Z. Galazka, G. Wagner, V. Wheeler, M. Tadjer, K. Goto, and V. Darakchieva, “Longitudinal phonon plasmon mode coupling in β-Ga2O3,” Applied Physics Letters 114, 102102 (2019) https://doi.org/10.1063/1.5089145.

67M. V. Fischetti, D. A. Neumayer, and E. A. Cartier, “Effective electron mobility in Si inversion layers in metal-oxide-semiconductor systems with a high-κ insulator: The role of remote phonon scattering,” Journal of Applied Physics 90, 4587–4608 (2001) https://doi.org/10.1063/1.1405826.

68A. Dyson and B. Ridley, “Phonon-plasmon coupled-mode lifetime in semiconductors,” Journal of Applied Physics 103, 114507 (2008).

69K. Diff and K. F. Brennan, “Theory of electron-phonon-scattering rate in highly doped bulk semiconductors,” Journal of Applied Physics 69, 3079–3103 (1991) https://doi.org/10.1063/1.348574.

70K. Björck, “Numerics of gram-schmidt orthogonalization,” Linear Algebra and Its Applications 197, 297–316 (1994).

71K. Hess, Monte Carlo device simulation: full band and beyond, Vol. 144 (Springer Science & Business Media, 2012).

72H. Jung, K. Taniguchi, and C. Hamaguchi, “Impact ionization model for full band Monte Carlo simulation in GaAs,” Journal of Applied Physics 79, 2473–2480 (1996).

73C. Jungemann, S. Keith, M. Bartels, and B. Meierzhanov, “Efficient full-band Monte Carlo simulation of silicon devices,” IEEE Transactions on Electronics 82, 870–879 (1999).

74T. Kunikyo, M. Takenaka, Y. Kamakura, M. Yamaji, H. Mizuno, M. Morifuji, K. Taniguchi, and C. Hamaguchi, “A Monte Carlo simulation of anisotropic electron transport in silicon including full band structure and anisotropic impact-ionization model,” Journal of Applied Physics 75, 297–312 (1994).

75S. Tyaginov, I. Starkov, O. Treibl, J. Cervenka, C. Jungemann, S. Carniello, J. M. Park, H. Enichlmair, M. Karner, C. Kernstock, et al., “Hot-carrier degradation modeling using full-band Monte-Carlo simulations,” in 2010 17th IEEE International Symposium on the Physical and Failure Analysis of Integrated Circuits (IEEE, 2010) pp. 1–5.

76N. Fitzer, A. Kuligk, R. Redmer, M. Städele, S. M. Goodnick, and W. Schattke, “Full-band Monte Carlo simulations of high-field electron transport in GaAs and InAs,” Physical Review B 67, 201201 (2003).

77M. V. Fischetti and S. E. Laux, “Monte Carlo study of electron transport in silicon inversion layers,” Physical Review B 48, 2244 (1993).

78D. Dolgos, H. Meier, A. Schenk, and B. Witzgall, “Full-band Monte-Carlo simulation of single photon avalanche diodes,” in 2013 IEEE Photonics Conference (IEEE, 2013) pp. 360–361.