Calculation of electron impact ionization co-efficient in β-Ga_2O_3

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Monoclinic β-Ga_2O_3 field effect transistors (FETs) have been recently explored for power electronics application [1, 2] due to its large bandgap, and the availability of native substrates. Quantitative impact ionization coefficient (α) values are required to accurately predict the achievable breakdown voltages in these devices. Here, we first report the theoretical calculation of the electron impact ionization co-efficient in β-Ga_2O_3 by numerically evaluating the electron distribution function at high electric fields using Baraff's method [3]. We have included acoustic deformation potential (ADP) scattering, impurity scattering (IS), polar optical phonon (POP) scattering, and impact ionization (II) scattering in our calculations. Non-polar optical phonons are found to have negligible effects. Cheynoweth exponential fit of the impact ionization coefficient is extracted that can be used in device simulators to optimize the device design for high breakdown voltages.

Baraff's method calculates the electron distribution function (*M(E)*) using the integral form of Boltzmann's transport equation (BTE) including energy dependent scattering rates [3]. The advantage of this method over Monte Carlo techniques is the reduced simulation time. We have included POP scattering in the calculation of electron distribution function, which was not considered in ref [3]. We calculate the saturation velocity (2.42×10^7cm/s) and mean free path (14.5 Å) in β–Ga_2O_3 using lucky electron drift model [4] and this mean free path is used for the rest process. The materials parameters considered in the calculation is given in Table I [5]. We have assumed a parabolic conduction band with no contribution of higher order bands to impact ionization. For ADP scattering, GaN parameters were used, since there is no elastic property data is available for Ga_2O_3 in literature. However, at high energies required to cause ionization, ADP scattering has negligible contribution to the electron energy distribution.

To calculate *M(E)*, electrons are first introduced with zero energy at $z = 0$, in a semiconductor region with a uniform electric field (F). They gain energy from the electric field ($q.F.z$), while different electron scattering mechanisms reduce the energy. The relative scattering cross-sections ($r = \sigma_i/\sigma_{total}$) of different mechanisms with energy is obtained from the calculated scattering rates of ADP, POP, IS and II. As seen in Fig. 1, the POP emission is the dominant scattering mechanism in reducing the energy of electrons for electron energy $E > E_R$ (phonon energy). Impact ionization scattering becomes active for energies beyond the threshold energy (E_I). E_I [6] is calculated to be 4.9 eV assuming a heavy hole mass ($m_h > 3m_0$). In the high field region, the dominant energy distribution mechanisms are the energy gained from electric field, POP emission, and impact ionization. It is sufficient to consider these for impact ionization calculations.

Now the probability an electron at an initial energy E' will reach to a final energy E is the joint probability of emitting n phonons and drifting a distance $(E - E' + nE_R)/qF$. This probability decreases rapidly with increasing n, converging for a given final energy. Evaluating this probability as a function of final energy gives *M(E)*. The distribution function multiplied by the density of states gives the total number of electrons at a given energy ($n_e(E)$). As seen in Fig. 2, at high electric fields the electron density function converges to a Maxwellian form. The impact ionization collision density is the product of the distribution function and the cross section of impact ionization. Fig. 3 shows the calculated normalized impact ionization collision density for Ga_2O_3 for different electric fields. Fig.4 shows the calculated expectation value of the energy (E_{avg}) of an electron and the average number of phonons (n_{avg}) it has emitted before being absorbed by impact ionization. The average distance (z_{avg}) an electron has travelled before being absorbed is given by $(E_{avg} + n_{avg}E_R)/qF$. The inverse of this distance, number of ionizations per unit length, is the impact ionization coefficient ($\alpha = 1/z_{avg}$). The calculated values of α as a function of electric field for Ga_2O_3 is plotted in Fig. 5. The inset gives a comparison of calculated vs experimental α for GaN [7], which shows the accuracy of the calculations. The calculated α for Ga_2O_3, fits the Cheynoweth exponential form, ($\alpha = a.exp(-b/F)$), with $a=2.5\times10^6$/cm and $b= 3.96\times10^7$ V/cm. The impact ionization generation rate ($G = \alpha.v_s$) is given in Fig 6.

Finally, we do a numerical simulation of the device in [1], in SILVACO ATLAS. Fig.7 shows the electric field in the device in the off state. The calculated ionization integral ($\int \alpha dx$) is approximately 0.525, which shows that the device is operating below the avalanche breakdown and higher breakdown voltages can be obtained.

In summary, we first report the calculated electron impact ionization co-efficient in Ga_2O_3. These calculated values would be useful in optimizing the Ga_2O_3 power devices for high breakdown voltages.

[1] Higashiwaki, Masataka, et al. *IEDM, 2013*
[2] Higashiwaki, Masataka, et al. *Applied Physics Letters* 103.12 (2013): 123511
[3] Baraff, Gene A. *Physical Review* 128.6 (1962): 2507
[4] Bringuier, E. *Physical Review B* 49.12 (1994): 7974.
[5] Liu, Bo, Mu Gu, and Xiaolin Liu. *Applied Physics Letters* 91.17 (2007): 172102-172102.
[6] Anderson, C. L., and C. R. Crowell *Phys. Rev. B5* (1972):2267
[7] Baliga, B. Jayant. *Semiconductor Science and Technology* 28.7 (2013): 074011.

Table I Properties of Ga_2O_3 used in calculation [5]

Property	Value
Effective mass (m_e)	$0.3m_0$
Bandgap (E_g)	4.9 eV
POP energy (E_R)	100 meV
Dielectric constant (static)	10
Dielectric constant (HF)	3.57

Ionization threshold, $E_I = \frac{2+\gamma}{1+\gamma} E_g$; $\gamma = \frac{m_h}{m_e}$ [6]

$$\frac{1}{\tau_{II}(E)} = \frac{m_e^3 e^4}{2\epsilon^2 h^2 m_h^2}\left(1+\frac{m_h}{m_0}\right)\left(\frac{E-E_I}{E_I+E_D}\right)^2 u(E-E_I);\ E_D = \frac{h^2 q_D^2}{8\pi^2 m_h};$$

$1/\tau_{II}$ is impact ionization scattering rate, q_D is the Debye wave vector

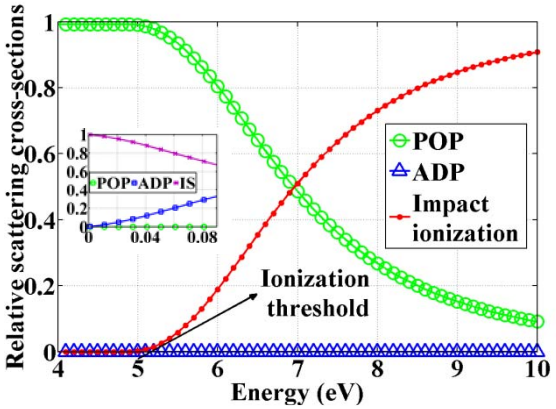

Figure 1: Relative cross-section of different scattering mechanisms (considering energy relaxation times) (Inset) Relative cross section of scatterings at low energies.

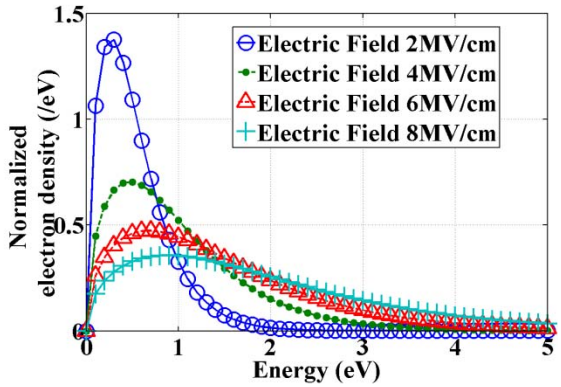

Figure 2: Calculated non-equilibrium normalized electron density for different electric fields.

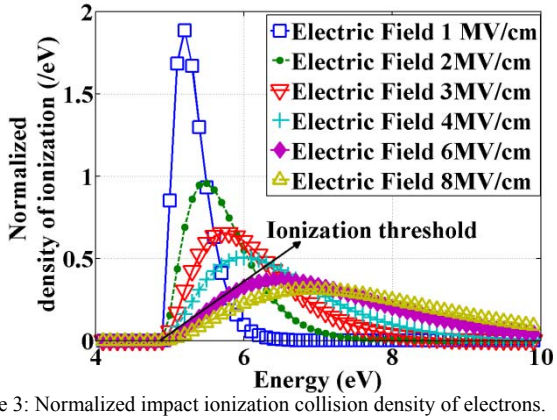

Figure 3: Normalized impact ionization collision density of electrons.

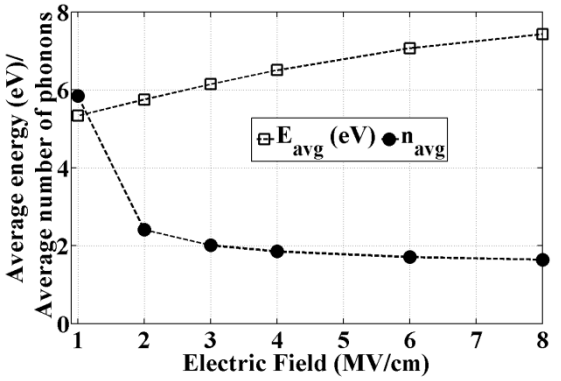

Figure 4: Average energy (E_{avg}) and average number of phonons (n_{avg}) emitted by an electron before ionization.

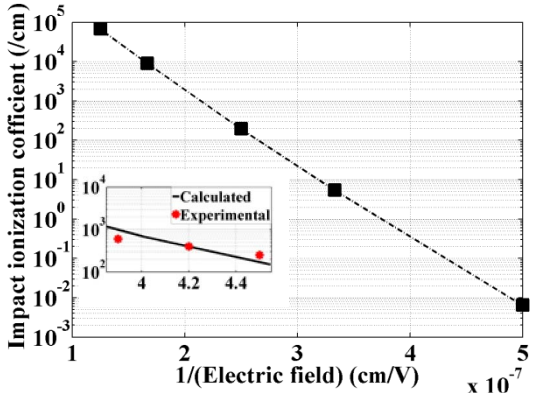

Figure 5: Impact ionization coefficient for different electric fields (Inset) Comparison of calculated vs experimental [7] α for GaN.

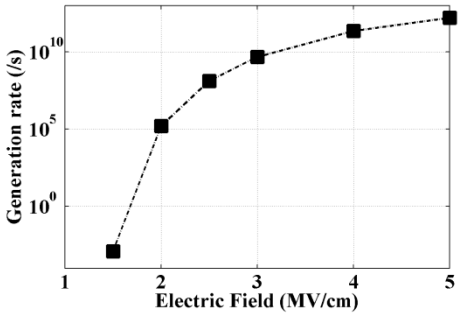

Figure 6: Generation rate of electrons at different electric fields

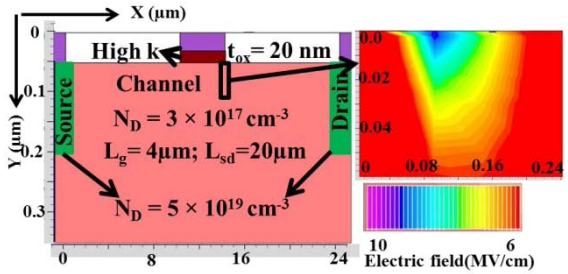

Figure 7: Simulated electric field profile of the Ga_2O_3 device demonstrated in [1] under a drain bias of 400 V and a gate bias of -30V.