Electron momentum relaxation rates via Frohlich interaction with polar-optical-phonons in bulk wurtzite gallium nitride

Kihoon Park,[1,2] Michael A. Stroscio,[3] and Can Bayram[1,2]

[1]*Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Illinois 61801, USA*
[2]*Micro and Nanotechnology Laboratory, University of Illinois at Urbana-Champaign, Illinois 61801, USA*
[3]*Department of Electrical and Computer Engineering, University of Illinois at Chicago, Chicago, Illinois 60607, USA*

Here, we present a formalism for calculating electron scattering rates and momentum relaxation rates due to interaction with polar-optical-phonons in bulk wurtzite gallium nitrides. The formalism is established based on the dielectric continuum model and the uniaxial model. Relaxation rates are calculated as a function of electron incident angle and initial energy. We report that the total momentum relaxation rates as well as the scattering rates are mostly determined by the longitudinal optical phonon modes. Electron incident angle variation shows almost no effect on interaction with longitudinal-optical-like phonon modes. In contrast, for transverse-optical-like phonon modes, both scattering rates and momentum relaxation rates show up to a factor of 1.8 difference near the emission threshold energy, as the angle varies from 0 to π/2 from the *c* axis.

I. INTRODUCTION

Gallium nitride (GaN) based heterostructure high electron mobility transistors (HEMTs) are ideal for high-power and high-frequency applications due to the excellent material properties of GaN such as high breakdown field (3.3 MV/cm), high saturation velocity (2.5×10^7 cm/s), high thermal and chemical stability. Studies have shown that up to 40 W/mm[1] power output is achievable with the development of GaN-based power transistors. Despite of these advantages, recent works show that these devices are thermally limited. For example, mismatch of the coefficient of thermal expansion (CTE) and temperature limited mobility are reasons suspected for the GaN-based HEMT current characteristics degradation at high voltages. As optical-phonon emission is known as the principal energy relaxation process of hot electrons in gallium nitride, the investigation of the interaction between electrons and polar-optical-phonons is critical in understanding this problem.

In this paper, we provide a formalism for the calculation of the incident angle and energy dependent electron scattering, momentum relaxation and present results obtained by numerical calculation.

II. FORMALISM AND RESULTS

We start from the solution of Loudon's model for frequencies of extraordinary phonons in uniaxial polar crystals[2]:

$$\omega_{LO}^2 = \omega_{zL}^2 \cos^2\theta + \omega_{pL}^2 \sin^2\theta ,$$

$$\omega_{TO}^2 = \omega_z^2 \sin^2\theta + \omega_p^2 \cos^2\theta ,$$

where θ is the angle between the phonon wave vector **q** and the *c* axis, and the subscripts *z* and *p* indicate directions parallel and perpendicular to the *c* axis, respectively.

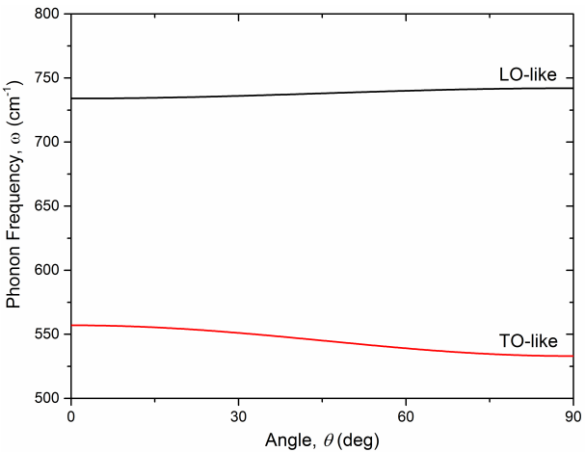

Figure 1. The longitudinal optical (LO) like and transverse optical (TO) like phonon frequencies as a function of angle between the phonon wave vector **q** and *c* axis in bulk wurtzite GaN.

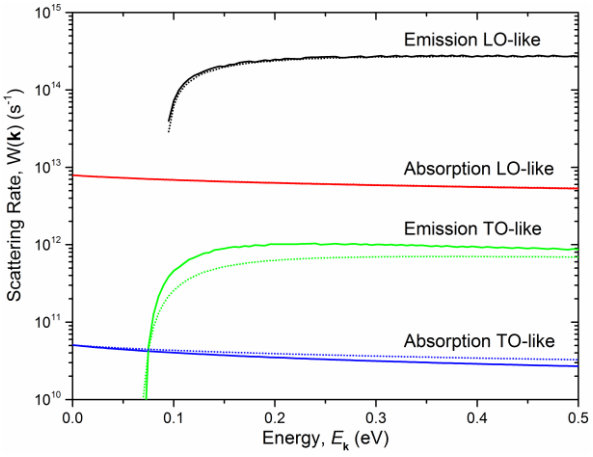

Figure 2. The electron energy variation of scattering rates with LO-like and TO-like phonon modes. Three different electron incident angles, θ_k is 0 (solid line) and π/2 (dotted line), are shown together.

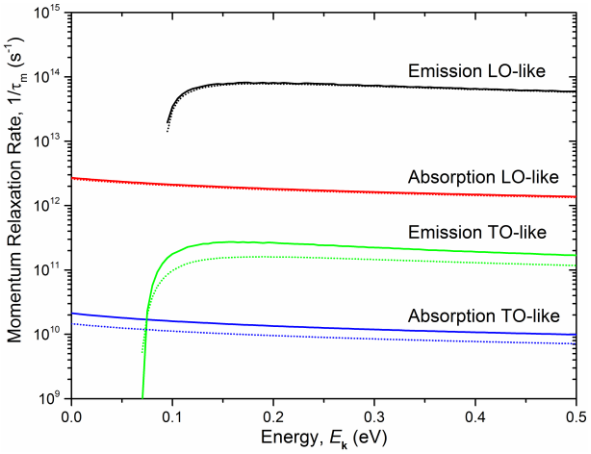

Figure 3. The electron energy variation of momentum relaxation rates for LO-like and TO-like phonon mode scattering.

The phonon frequencies used in the numerical calculations are taken from experimental results[3]: ω_{zL} = 734 cm^{-1} and ω_z = 533 cm^{-1} for A_1 LO and TO phonons, ω_{pL} = 742 cm^{-1} and ω_p = 557 cm^{-1} for E_1 LO and TO phonons, respectively. Figure 1 shows the angular variation of the LO-like and TO-like phonon frequencies.

The normalized electron–optical-phonon Hamiltonian for uniaxial material is given as[4]

$$H = \sum_{\mathbf{q}} \sqrt{\frac{2\pi e^2 \hbar}{V\omega}} \Omega^{1/2}(\theta) \frac{1}{q} e^{i\mathbf{q}\cdot\mathbf{r}} \left(a_{\mathbf{q}} + a_{-\mathbf{q}}^{*}\right)$$

such that

$$\Omega^{-1}(\theta) = \frac{\left(\varepsilon_{\perp}^{0} - \varepsilon_{\perp}^{\infty}\right)\omega_{\perp}^{2} \sin^2\theta}{\left(\omega_{\perp}^{2} - \omega^2\right)^2} + \frac{\left(\varepsilon_{z}^{0} - \varepsilon_{z}^{\infty}\right)\omega_{z}^{2} \cos^2\theta}{\left(\omega_{z}^{2} - \omega^2\right)^2}$$

The electron scattering rate due to Frohlich interaction is obtained by the Fermi golden rule as

$$W(\mathbf{k}) = \frac{e^2\sqrt{m^*}}{2\sqrt{2}\pi\hbar} \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \left(n_{ph} + \frac{1}{2} \pm \frac{1}{2}\right) \times \frac{\Omega(\theta)}{\omega} \frac{\sigma\sqrt{E_{\mathbf{k}}\cos^2\phi' \mp \hbar\omega}}{\left(\sqrt{E_{\mathbf{k}}\cos^2\phi' \mp \hbar\omega} + q_0\right)^2}$$

where ϕ' is the angle between the phonon wave vector **q** and the initial electron wave vector **k**. For the case of emission (upper signs), σ is equal to 2 when $E_{\mathbf{k}}\cos^2\phi' > \hbar\omega$, and for the case of absorption (lower signs) σ=1. Here, we have included a screening factor of q_0 = 8×10^{-12} to facilitate efficient numerical integration in the case of emission when $E_{\mathbf{k}}\cos^2\phi' \approx \hbar\omega$. Figure 2 shows the electron scattering rates as a function of electron incident energy. LO-like phonon mode scattering shows no $\theta_{\mathbf{k}}$ angle dependence whereas TO-like scattering shows up to a factor of 1.8 difference near the emission threshold energy.

The momentum relaxation of electrons is expressed as

$$\frac{1}{\tau_m^{e}} = -\frac{e^2\sqrt{m^*}}{\sqrt{2}\pi\hbar} \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \left(n_{ph} + 1\right) \times \frac{\Omega(\theta)}{\omega} \frac{\cos^2\phi' \sqrt{E_{\mathbf{k}}\cos^2\phi' - \hbar\omega}}{\left(\sqrt{E_{\mathbf{k}}\cos^2\phi' - \hbar\omega} + q_0\right)^2}$$

$$\frac{1}{\tau_m^{a}} = \frac{e^2\sqrt{m^*}}{2\sqrt{2}\pi\mathrm{h}} \grave{O}_0^{2\pi} d\mathbf{f} \grave{O}_0^{\pi} \sin\theta d\theta \left(n_{ph}\right) \times \frac{\Omega(\theta)}{\omega} \frac{\cos^2\mathbf{f}\,\phi' + \cos\mathbf{f}\,\phi' \sqrt{\cos^2\mathbf{f}\,\phi' + \mathrm{h}\omega/E_{\mathbf{k}}}}{\sqrt{E_{\mathbf{k}}\cos^2\mathbf{f}\,\phi' + \mathrm{h}\omega}}$$

where the superscript *a* and *e* indicate the relaxation rates due to phonon absorption and emission, respectively. We have also included the screening factor q_0 for the case of phonon emission. Figure 3 shows the numerically calculated momentum relaxation rates as a function of electron initial energy due to LO-like and TO-like phonons. Note that the absolute values are taken for the emission rates. Similar to the scattering rates, small anisotropy is shown near the electron emission threshold energy.

III. CONCLUSIONS

Electron–optical-phonon scattering rates and momentum relaxation rates were calculated numerically as a function of incident angle and electron energy. LO-like phonon scattering shows no dependency on electron incident angle whereas TO-like phonon scattering exhibits a maximum of 80% anisotropy near $E_{\mathbf{k}} = \hbar\omega_{TO}$.

ACKNOWLEDGEMENT

Part of this work, supported by the Air Force Office of Scientific Research (AFOSR) through Young Investigator Program Grant FA9550-16-1-0224, was carried out in the Micro and Nanotechnology Laboratory, University of Illinois at Urbana-Champaign, IL, USA. Part of this work, supported by the Air Force Office of Scientific Research (AFOSR) Grant FA9550-16-1-0227, was carried out at the University of Illinois at Chicago, IL, USA.

REFERENCES

[1] Y.-F. Wu, et al., in Proceedings of 2006 64th Device Research Conference, June 2006, pp. 151-152.
[2] R. Loudon, Adv. Phys. **13**, 423 (1964).
[3] V. Y. Davydov, et al., Phys. Rev. B, **65**, 125203 (2002).
[4] M. A. Stroscio and M. Dutta, *"Phonons in Nano-structures,"* Cambridge University Press (2001).