Closing the "10-100 eV Gap" for Electron Thermalization in GaN Devices from First Principles

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Introduction

Since the launch of Sputnik I in 1957, human presence in space has expanded greatly, and with it the demand for durable and reliable technologies, capable of operating in environments with high levels of radiation exposure. As a result, increased attention has been placed on radiation effects on electronic devices [1,2,3], and it has become necessary to improve the accuracy of computational models used to simulate these effects. The present work concentrates on radiation effects in GaN but can be extended to any material of interest.

The major focus of this work is to study theoretically the energy-loss processes that control the thermalization of hot electrons and/or electron-hole pairs that are generated by high-energy radiation in semiconductors. Current knowledge and capabilities cover both the high-energy range (energies above ~100 eV), where nuclear/particle-physics computational tools have been successfully applied [4], and the lower-energy range (below ~10 eV), which has been studied extensively by the electronic-device community [5]. The processes that control electron and hole thermalization in the intermediate range are poorly known (the "10-100 eV gap"), with only a few studies (which used a free-electron model) showing losses to plasmons being the dominant process [6].

Theoretical Models

As electrons thermalize from the high-energy, free-electron regime into this intermediate range, they begin to feel the effects of the band structure, necessitating a first-principles calculation. Using the density functional theory (DFT) package Quantum ESPRESSO, we obtain the electronic band structure for 150 bands, reaching energies above 100 eV. We also calculate the phonon dispersion and the associated electron-phonon matrix elements to evaluate the electron- and hole-phonon scattering rates via Fermi's Golden Rule (Fig. 1).

To deal with losses to plasmons and impact ionization, we utilize time-dependent DFT to calculate the dynamic dielectric function, $\varepsilon(\mathbf{q},\omega)$. Employing the fluctuation-dissipation theorem, we calculate the energy-loss rate (ELR), $1/\tau_n(\mathbf{k})$, of an electron in conduction band n with wavevector $\mathbf{k}$, in terms of the imaginary part of the inverse dielectric function [7,8,9]:

$$\frac{1}{\tau_n(\mathbf{k})} = \frac{2\pi}{\hbar}\sum_{n'}\int \frac{\mathrm{d}\mathbf{q}}{(2\pi)^3}\frac{e^2\hbar}{q^2}\int\frac{\mathrm{d}\omega}{2\pi}\,\mathrm{Im}\left[\frac{-1}{\varepsilon(\mathbf{q},\omega)}\right]\begin{Bmatrix} n(\omega) \\ 1+n(\omega)\end{Bmatrix}\delta[E_n(\mathbf{k}) - E_{n'}(\mathbf{k}+\mathbf{q}) \pm \hbar\omega]\,, \qquad (1)$$

where $n(\omega)$ is the Bose-Einstein distribution function (Fig. 1). The loss function $\mathrm{Im}[-1/\varepsilon(\mathbf{q},\omega)]$ exhibits peaks (shown in Fig. 2), associated with either plasmon losses or impact ionization. Plasmon peak positions yield the dispersion of the valence *sp*- and *d*-electron plasmons and their widths yield the plasmon lifetimes (Fig. 3).

Monte Carlo Simulation

Using the above results in a full-band Monte Carlo program, we study the time dependence of the thermalization of electrons and high-energy hole generation in GaN. Using a synchronous ensemble, electrons are allowed to advance through time with interaction mechanisms and subsequent final states being chosen stochastically. Electron-hole pairs are generated when impact ionization or plasmon emission is chosen. Thanks to the extremely short plasmon lifetimes (Fig. 3, bottom frame), we have assumed their immediate decay into electron-hole pairs. Full thermalization is achieved in ~1 ps (Fig. 4). Hot electrons produce pairs with an average energy of ~9.4 eV/pair, and spread ~10^{-7} m from their starting positions (important for device simulation).

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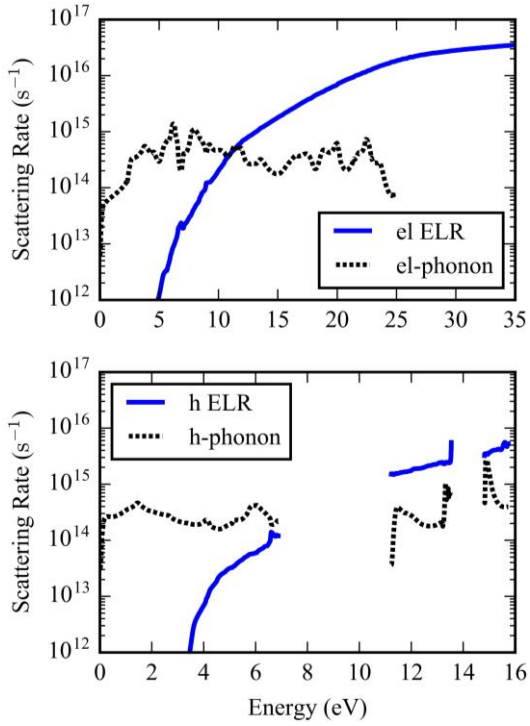

Fig. 1. Top: Electron-phonon scattering rate and electron energy-loss rate (ELR) plotted together. **Bottom:** Hole-phonon scattering rate and hole ELR. Gaps correspond to energy gaps in the valence bands.

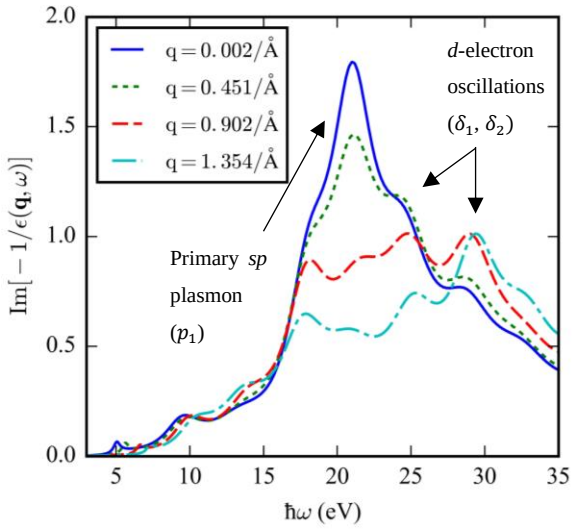

Fig. 2. Imaginary part of the inverse dielectric function of GaN calculated using the DFT package Quantum ESPRESSO. The function $\mathrm{Im}[-1/\varepsilon(\mathbf{q},\omega)]$ is plotted vs. the energy, $\hbar\omega$, for the indicated values of $\mathbf{q}$. Plasmon peaks (p_1, δ_1, and δ_2) are indicated.

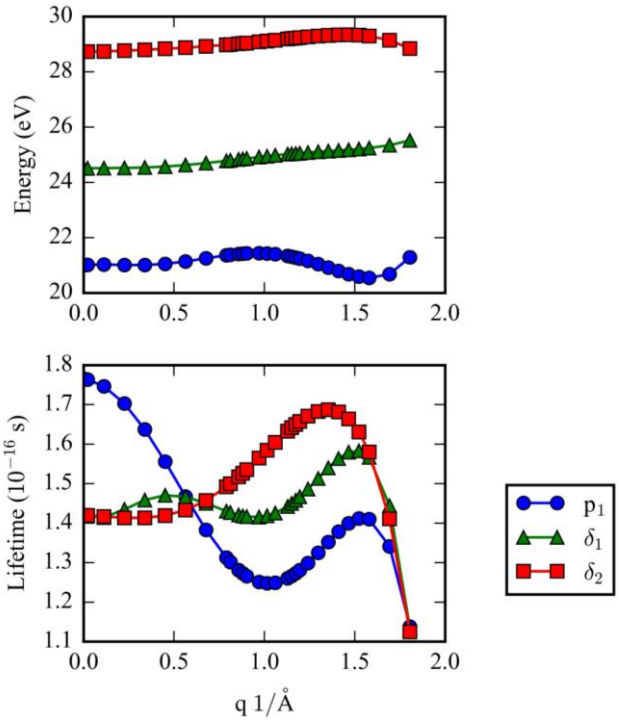

Fig. 3 Plasmon dispersion (top) and lifetime (bottom) obtained from the position and width of the quasi-Lorentzian peaks (p_1, δ_1, and δ_2) shown in Fig. 2.

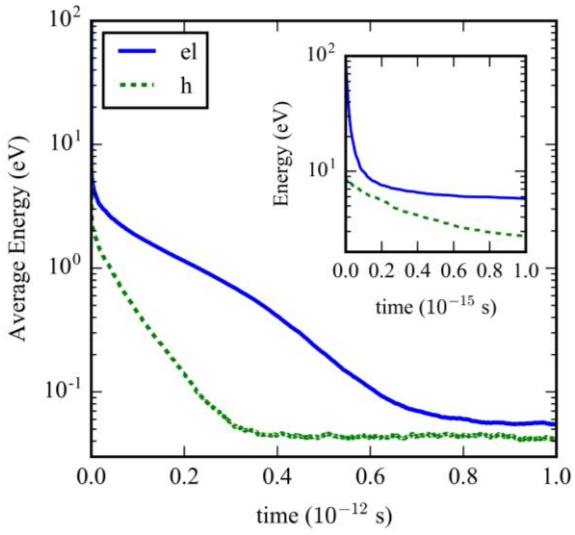

Fig. 4. Relaxation of electrons from a kinetic energy of 100 eV shown with the average energy of the generated holes throughout the thermalization process. **Embedded figure:** the first 10^{-15} s of the simulation.