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

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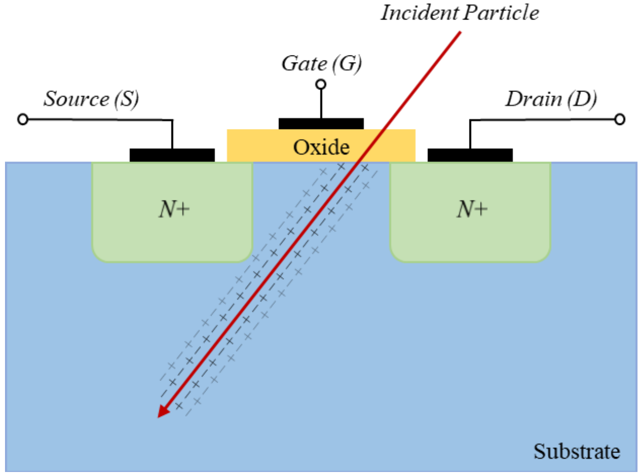
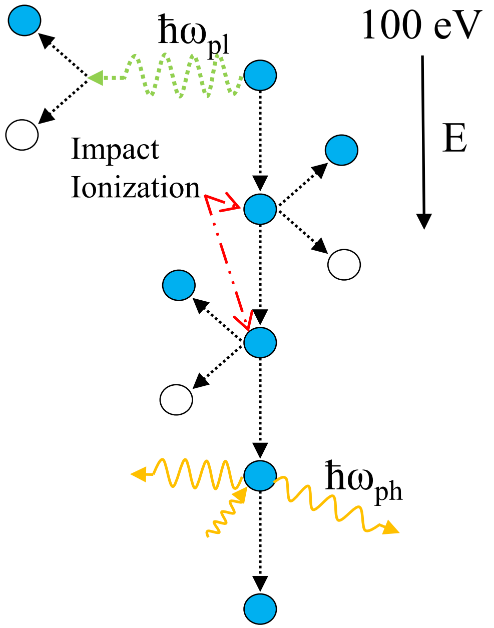
Introduction



- Ionizing radiation effects → high-E charge carriers
  - Nuclear/particle physics community: Binary-collision codes [1,2]
    - Good down to ~ 100 eV [3]
    - Band structure effects?
  - Electronic device community: full-band Monte Carlo [4]
    - Region below ~ 10 eV = well studied
  - Intermediate energy range: ~ 10-100 eV
    - Energy-loss processes not well understood [5]
- This work → study energy-loss processes from first principles
  - Close the gap
- Increasing popularity of WBG materials (GaN, SiC, β-Ga_2O_3, etc.)
  - Focus on GaN



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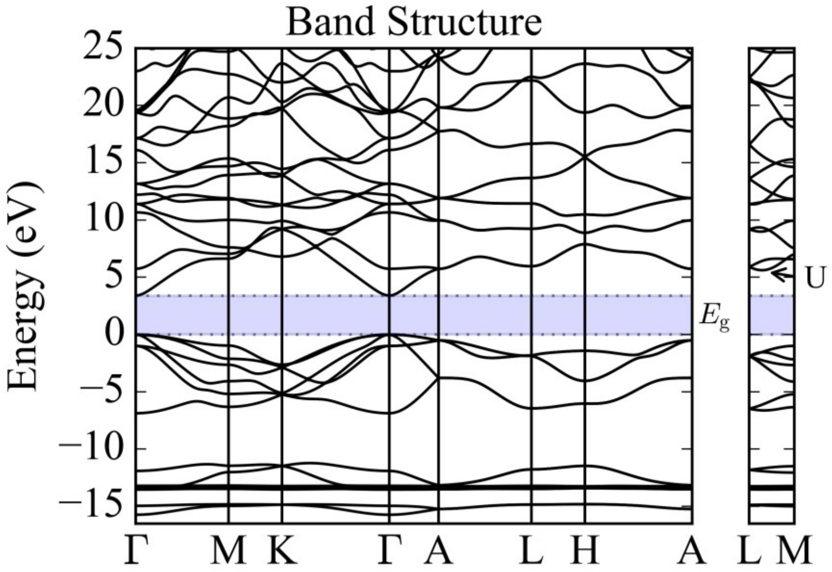
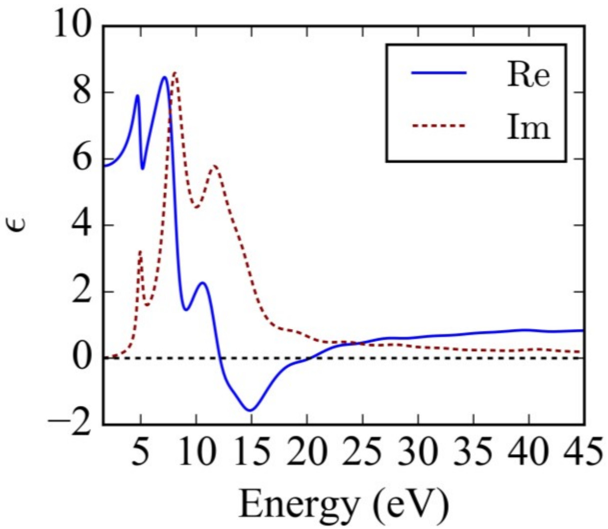
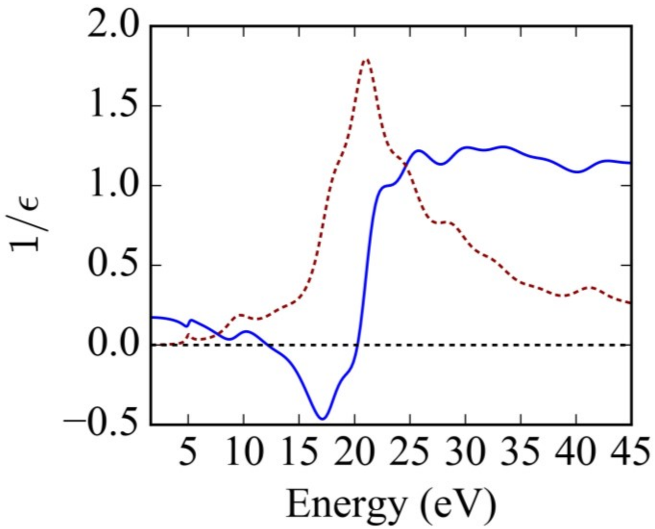
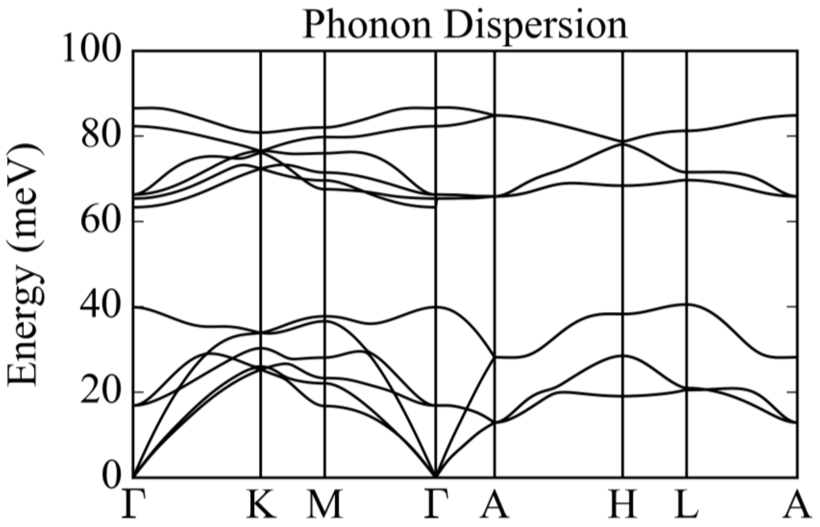
First Principles Calculations

- Use DFT and DFPT → *Quantum ESPRESSO* [1]
  - Band structure
  - Phonon dispersion
  - Dielectric function (TDDFT, *turboEELS* [2])
- EPW [3] → carrier-phonon matrix elements









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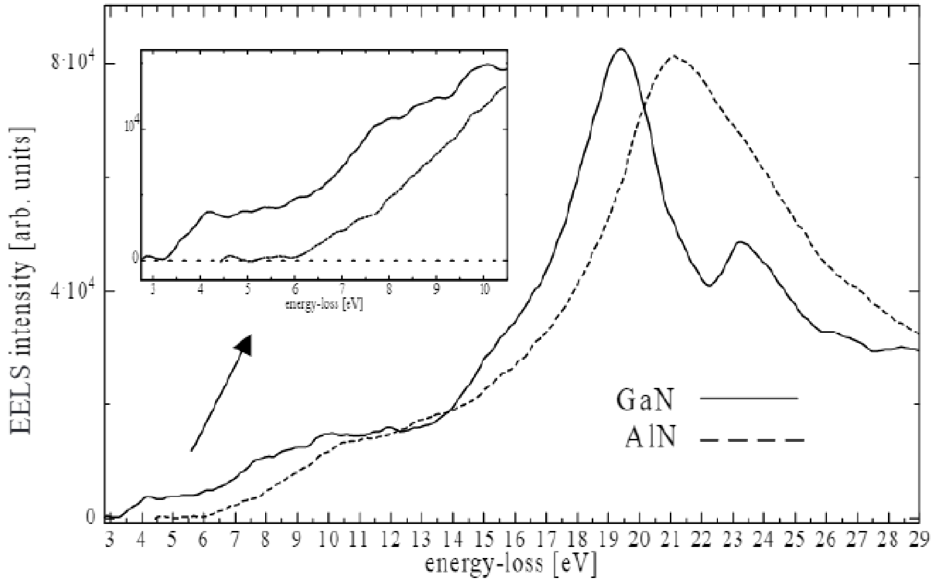
Scattering Rate Calculations

- Carrier-phonon scattering → use Fermi's Golden Rule (FGR):

$$\frac{1}{\tau_n^{(\eta)}(\mathbf{k})} = \frac{2\pi}{\hbar}\sum_{n'\mathbf{q}} \left|g_{nn'}^{\eta}(\mathbf{k},\mathbf{q})\right|^2 \left(N_{\mathbf{q}} + \frac{1}{2} \mp \frac{1}{2}\right) \delta\left[E_n(\mathbf{k}) - E_{n'}(\mathbf{k}\pm\mathbf{q}) \pm \hbar\omega_{\mathbf{q}}^{(\eta)}\right]$$

  - $N_{\mathbf{q}} = 1/(e^{(\hbar\omega_{\mathbf{q}}/k_B T)} - 1)$ (assuming T=300 K)
  - Evaluation of delta function done by Blöchl's tetrahedron method [1].
- Carrier energy-loss rate (ELR)
  - Electron energy loss spectroscopy (EELS)
    - Peaks = impact ionization and plasma excitations
  - Calculate total interaction rate using dielectric function (directly related to EEL cross section)
    - FGR and dissipation fluctuation theorem [2,3,4]:

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



Low-loss spectra of GaN and AlN [5]

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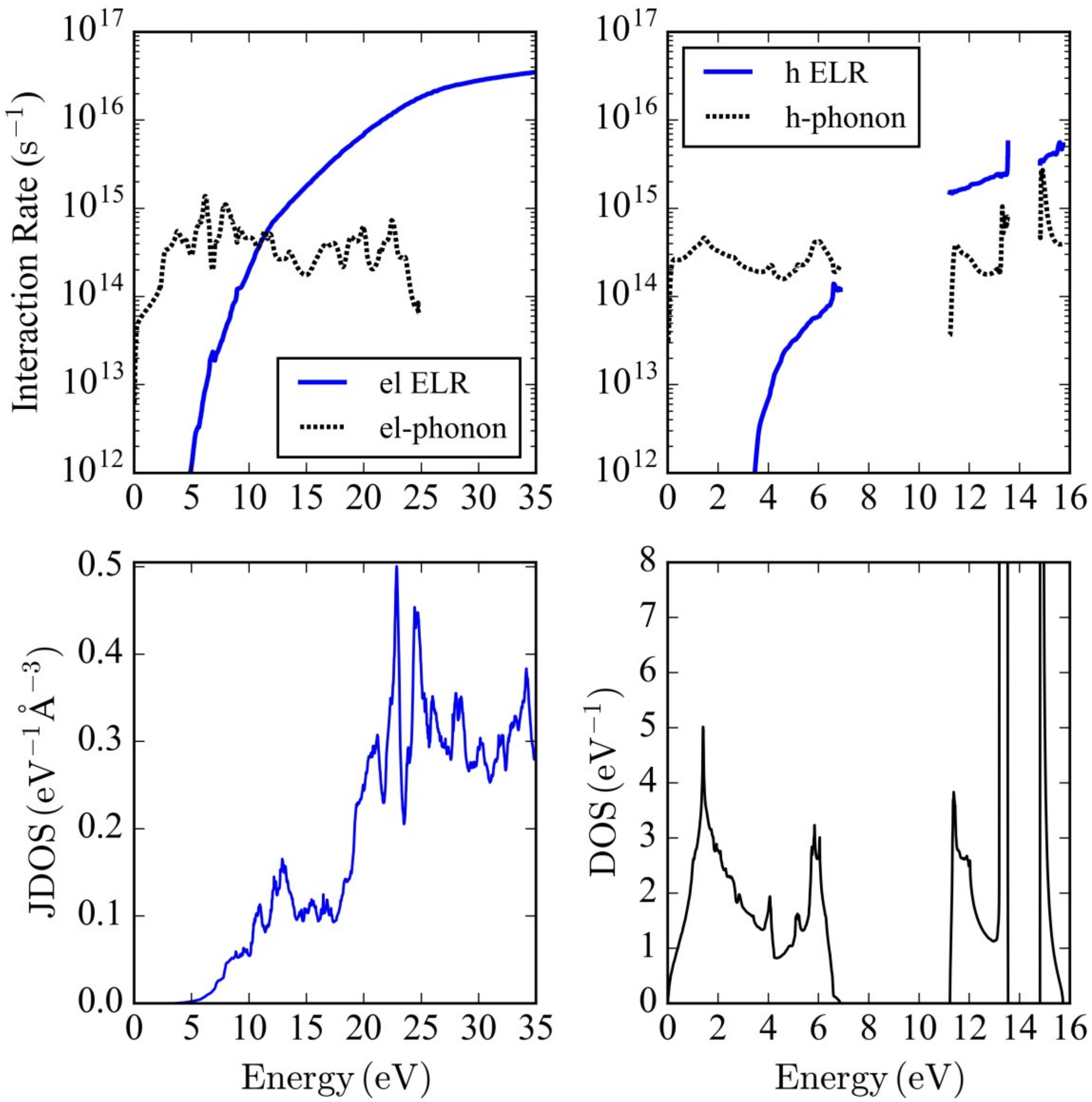
Scattering Rate Results

- Phonon scattering and ELR (top row)
- JDOS and VB DOS (bottom row)
- Electrons:
  - Phonon scattering dominant ≤ 10 eV
  - ELR flattens out at high energies
  - Rates driven to magnitude $> 10^{16}$ 1/s by dense *d* bands (see JDOS)
  - Quinn, Ferrell, Pines, Penn calculated rates of similar magnitude [1-4]
- Holes
  - Phonon scattering dominant for low E
  - Spikes at $\sim$13 and 15 eV from spikes in DOS for *d* bands



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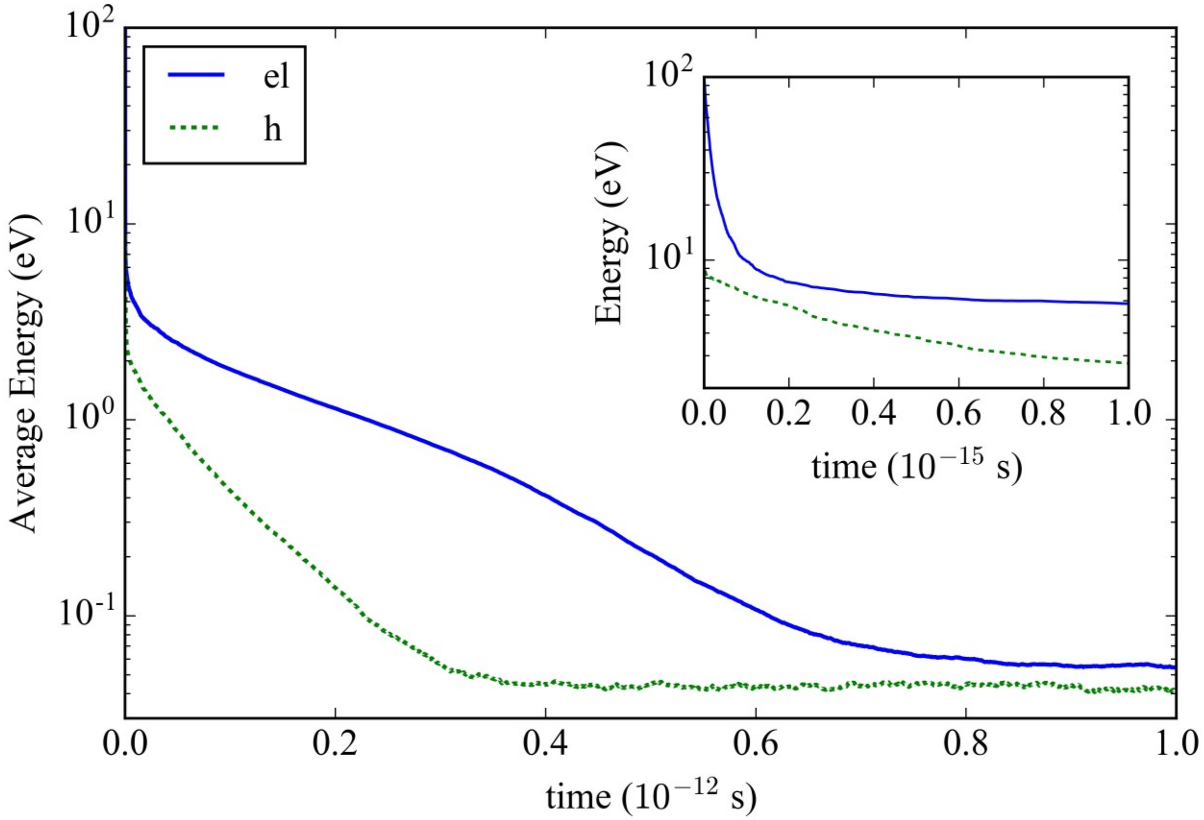
FBMC - Hot Electron Thermalization

- Solving BTE
  - Full band inclusion [1,2]
- Conditions: 0 field, 300 K
  - Inject 1000 electrons ($E\sim100\ eV$)
- Larger frame = Full thermalization, embedded frame = early stages
  - Rapid energy loss (t $< 10^{-16}$ s)
    - Plasmon emission/impact ionization
  - Thermalization rate decrease ($10^{-16} <$ t $< 10^{-14}$ s)
    - Impact ionization/phonon scattering
  - Roughly exponential decrease to thermal energy (t $> 10^{-14}$ s)
    - Phonon scattering
- Holes
  - No rapid initial decrease
  - Sharper slope (larger frame)
- Average energy per pair of $\sim$8.9 eV/pair [3,4]



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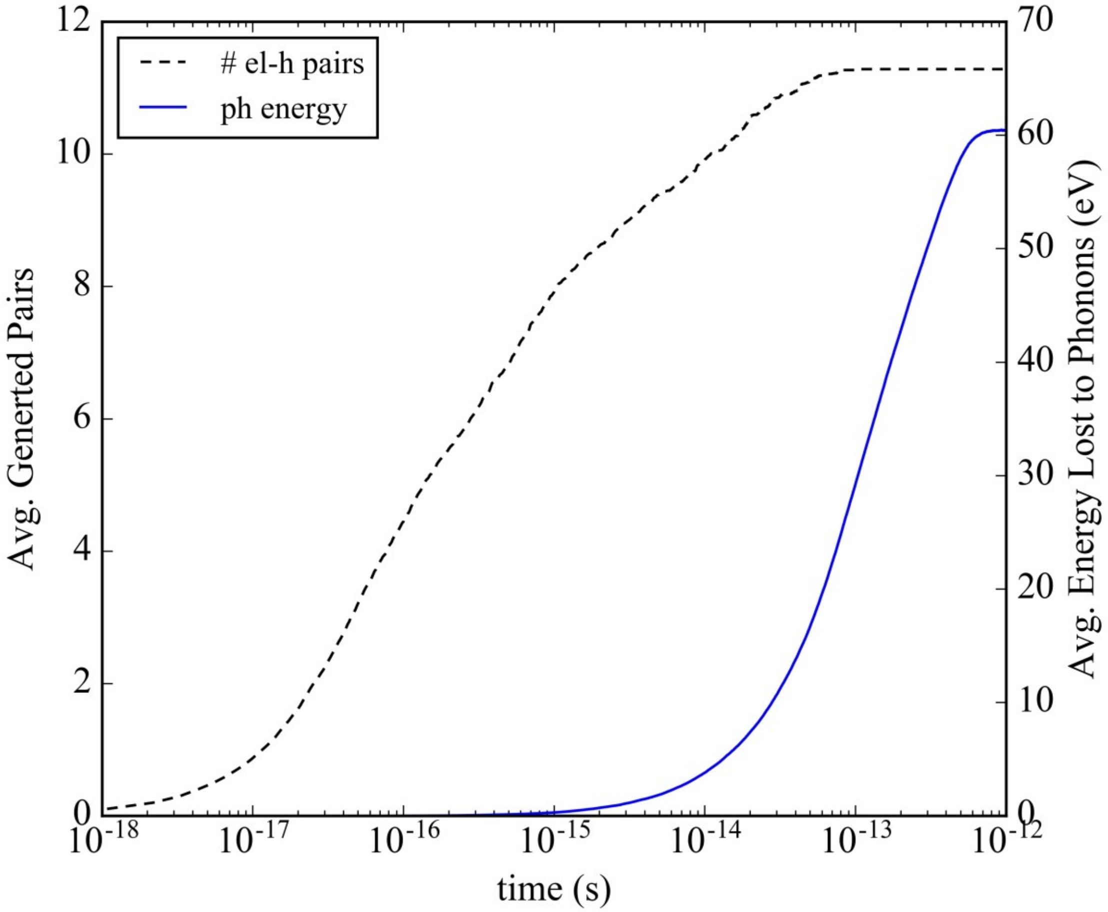
Where does the energy go?

- At first, E goes to pairs
- At $\sim 10^{-14}$ s, phonon emission increases significantly
  - Pair generation flattens
- Recombination [1]
- Temperature effects
  - Ignore, for now: assume low phonon density
  - No problems early on
  - May be a factor for $t > 10^{-13}$ s



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Conclusions

- Presented a first principles study of electron transport in “10-100 eV gap”
  - Includes band structure effects up to 100 eV
  - Studied plasmon and impact ionization in this energy regime
- Next steps…
  - Implement physics in device-level code
  - Include vacancies (radiation damage)
  - Simulate realistic streak
  - Investigate temperature effects

Thank you!

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