Thermalization of radiation-induced carriers in insulators and wide bandgap semiconductors and semiconductor devices (HEMTs)

(GaN, diamond, β-Ga_2O_3, Si, SiC,… for now)

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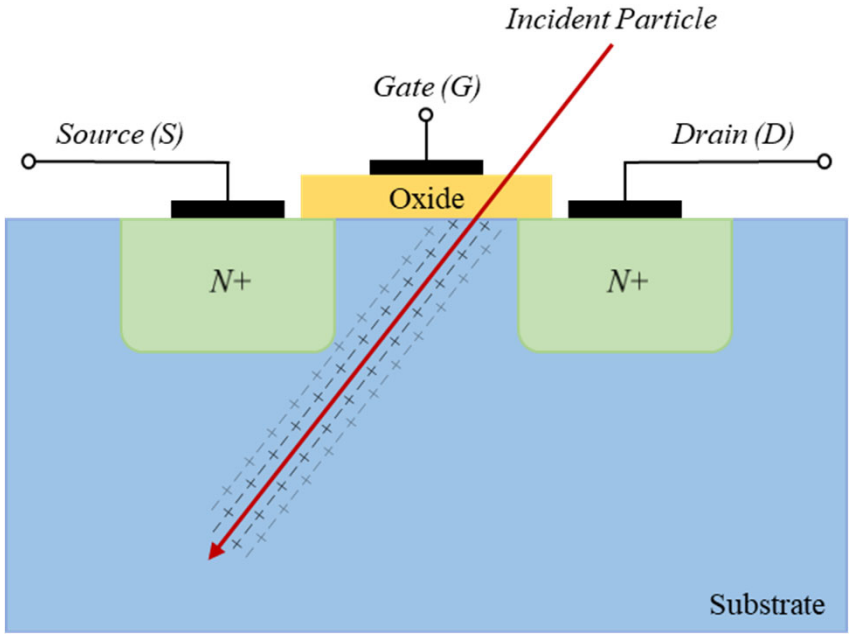
The problem

Simulate single-event effects/upsets (SEE/SEUs) in electron devices

- Basic ingredients
  1. Spatial and energetic distribution of the electron-hole (e-h) pairs after the (proton) strike
  2. Thermalization and diffusion of the e-h pairs
  3. Properties of possible precursor defects at interfaces/bulk (permanent damage)
- Present state of the art to obtain these ingredients
  1. High-energy binary collision Monte Carlo code (*e.g.*, Geant-4, MRED)
  2. Assume instantaneous complete thermalization + drift-diffusion
  3. Empirical cross sections and threshold/activation energies
- Our approach
  1. Use DTF below 100 eV (close the '10-100 eV gap')
  2. Consider e-h pair distributions from step 1 and use full-band Monte Carlo
  3. Cross sections and activation energies also from *ab initio* calculations



Outline

- Review and new results:
  1. Calculated energy-loss function (ELF) from DTF up to 100 eV
     Calculated rates for carrier-plasmon, carrier-phonon interactions and impact ionization
     - GaN, β-Ga_2O_3, C (diamond), Si, and SiC (fcc)
  2. Used full-band MC to study carrier relaxation (bulk)
     Used distributions after fast relaxation (~100 fs) as initial configuration in Monte Carlo device-simulation code: A GaN/AlGaN HEMT
     - Major coding work on Anduril
     - Test code to calculate hot-electron damage generation in a high-V_{DS}-stressed GaN/AlGaN HEMT (empirical cross section and threshold energy for defect creation)
     - Test code to calculate radiation-induced damage and current transient (upset) during an SEE
  3. Cross sections and activation energies from *ab initio* calculations; with Laura Nichols and Sok Pantelides (VU), and Xiaoguang Zhang (UF) – just starting
     - De-hydrogenation of V_{Ga}-H_3 complexes at the GaN-AlGaN interface of a p-channel HEMT

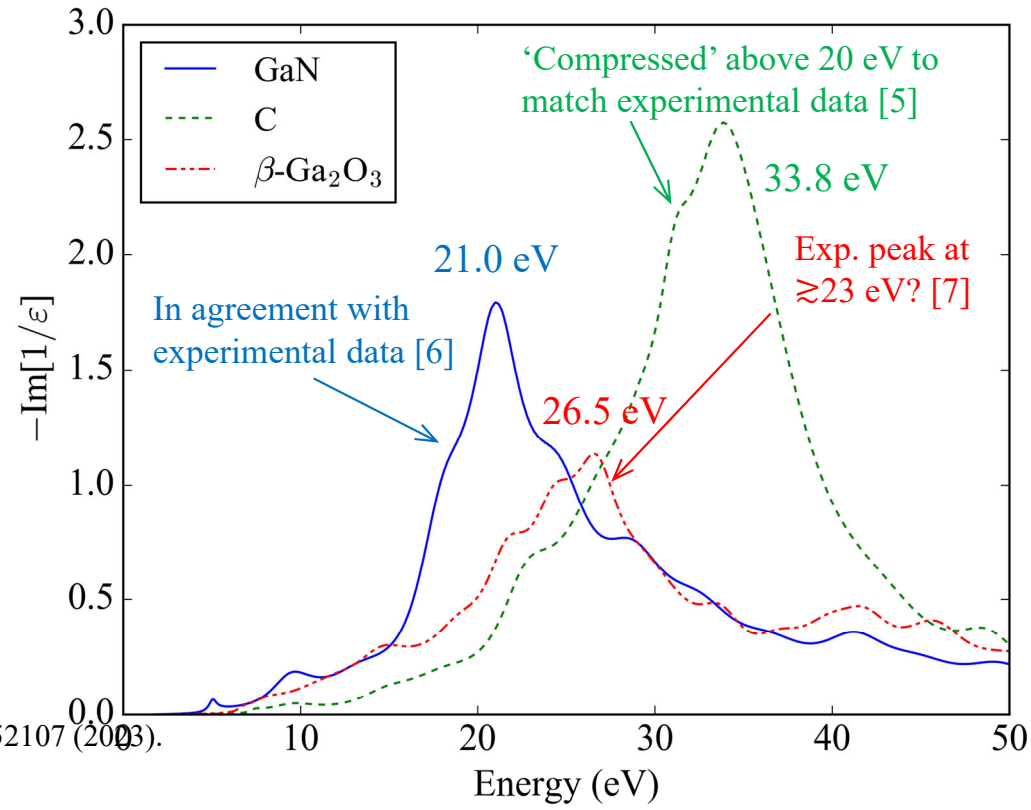
Summary of new results

1. Thermalization of 100 eV electrons in Si and SiC
2. Damage generated by hot electrons at the GaN-AlGaN interface of a HEMT stressed at high drain bias
3. Damage induced by 100 eV electrons in a GaN/AlGaN HEMT
4. Dehydrogenation of V_{Ga}-H_3 complexes at the GaN-AlGaN interface

Only "proof-of-concept" (or 'work in progress) for now.
Missing: 1. GaN hole transport in MC device code
2. Reliable information about defect precursors
3. Pair momentum distribution in the 'streak'
(… but probably already isotropic in ~100 fs)

First Principles Calculations [1]

- DFT and DFPT (*Quantum ESPRESSO* [2])
  - Band structure
    - "Scissor operator" to fit gap including also excitonic effects when significant (diamond)
  - Phonon dispersion
  - Dielectric function (TDDFT, *turboEELS* [3])
    - Plasmon emission and impact ionization from energy-loss (EL) function Im $\left(\frac{-1}{\epsilon(\mathbf{q},\omega)}\right)$
- EPW [4]: Carrier-phonon matrix elements
- Loss function:
  - Stronger peaks → higher plasmon emission rate
  - GaN and β-Ga_2O_3 plasmon energies lower than C → slower carrier thermalization



Calculated energy-loss functions for C (diamond), GaN (wurtzite) [1], and β-Ga_2O_3

[1] D. O. Nielsen *et al.*, Phys. Rev. B **108**, 155203 (2023); Appl. Phys. Lett. **123**, 252107 (2023).
[2] P. Giannozzi, *et al.*, J. Phys. Cond. Matt. **21**, 395502 (2009).
[3] I. Timrov, *et al.*, Comput. Phys. Commun. **196**, 460 (2015).
[4] S. Poncé, *et al.*, Comput. Phys. Commun. **209**, 116 (2016).
[5] J. Cañas *et al.* ," Appl. Surf. Sci. **461**, 93 (2018).
[6] R. Dhall, *et al.* , Appl. Phys. Lett. **112**, 061102 (2018).
[7] C. Fares *et al.*,. ECS J. Solid State Sci. Technol. **8**, Q3154 (2019) (Surface losses from REELS. Data only up to 25 eV).

Scattering Rates: Calculation [1]

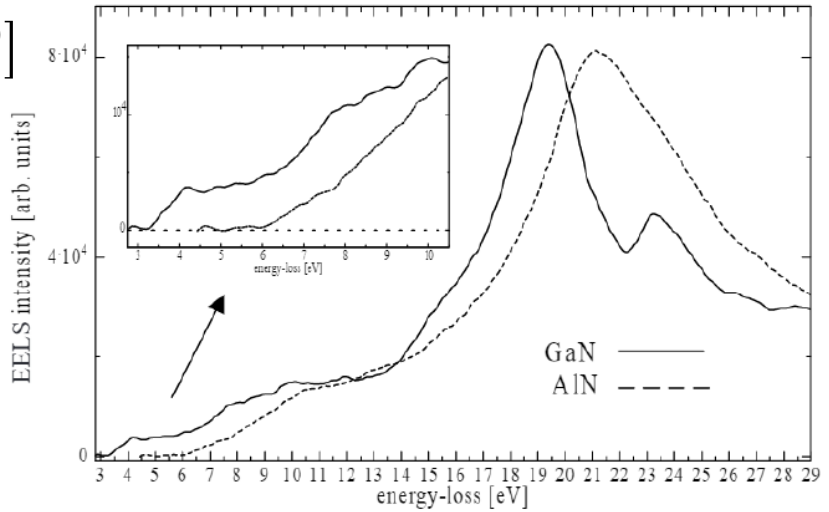
- Carrier-phonon scattering (Fermi's Golden Rule, FGR):

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

  - $N_{\mathbf{q}} = 1/(e^{(\hbar\omega_{\mathbf{q}}/k_BT)} - 1)$ (assuming T=300 K)
  - Evaluation of delta function done by Blöchl's tetrahedron method [2].

- Carrier energy-loss rate (ELR)
  - Electron energy loss spectroscopy (STM-EELS)
    - Peaks = impact ionization and plasma excitations (see figure)
  - Total rate using dielectric function (directly related to EEL cross section), FGR and dissipation fluctuation theorem [3-5]:

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



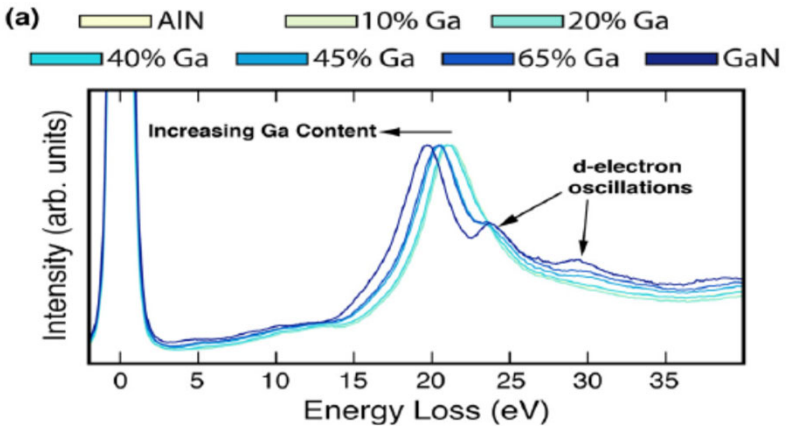
Experimental energy-loss spectra of GaN and AlN [6]

- Assume a low radiation-dose rate: Small density, no conduction-band el-el scattering, no heating

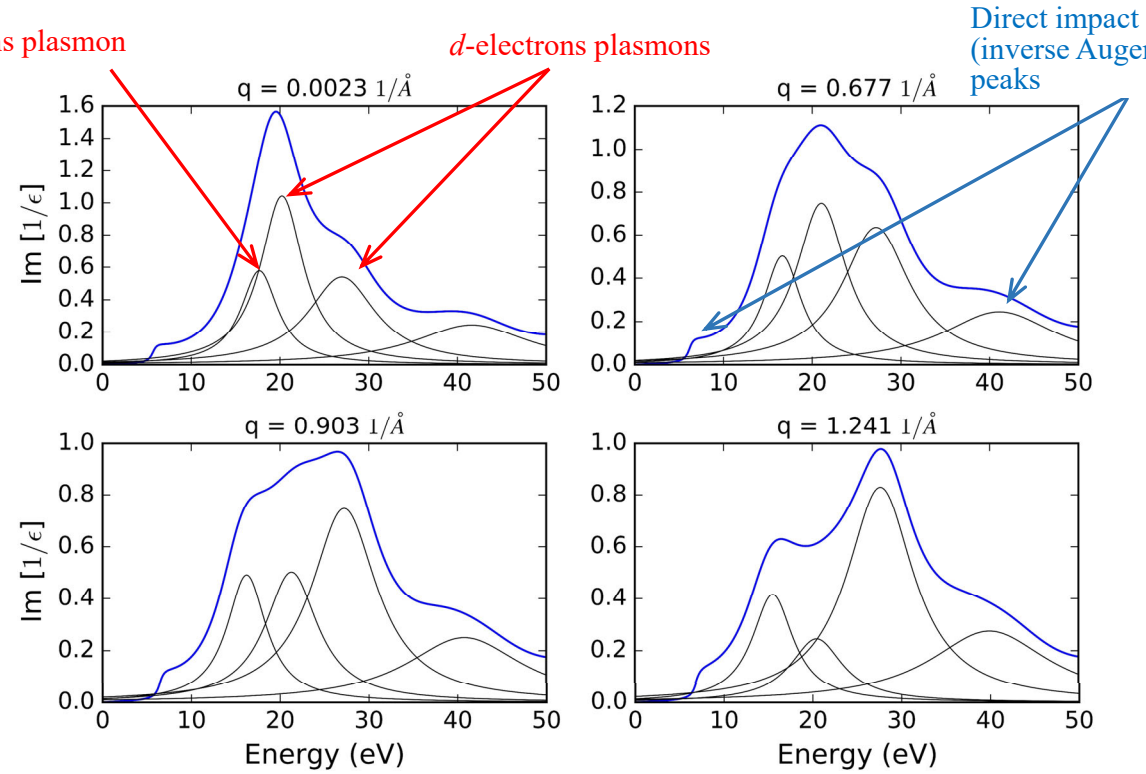
[1] D. O. Nielsen *et al*., Phys. Rev. B **108**, 155203 (2023)); Appl. Phys. Lett. **123**, 252107 (2023)..
[2] P. E. Blöchl, O. Jepsen, and O. K. Andersen, Phys. Rev. B **49**, 16223 (1994).
[3] P. Nozières and D. Pines, *Theory of Quantum Liquids*, Advanced Book Classics Series (Westview Press, Boulder, CO, 1999).
[4] H. Nyquist, Phys. Rev. **32**, 110 (1928)/
[5] H. B. Callen and T. A. Welton, Phys. Rev. **83**, 34 (1951).
[6] G. Brockt and H. Lakner, Micron **31**, 435 (2000).

The energy-loss function Im $\left[-\frac{1}{\varepsilon(\mathbf{q},\omega)}\right]$(GaN)

(from the RPA, finding plasmons and JDoS peaks via Lorentzian fits… just to understand, but academic*)



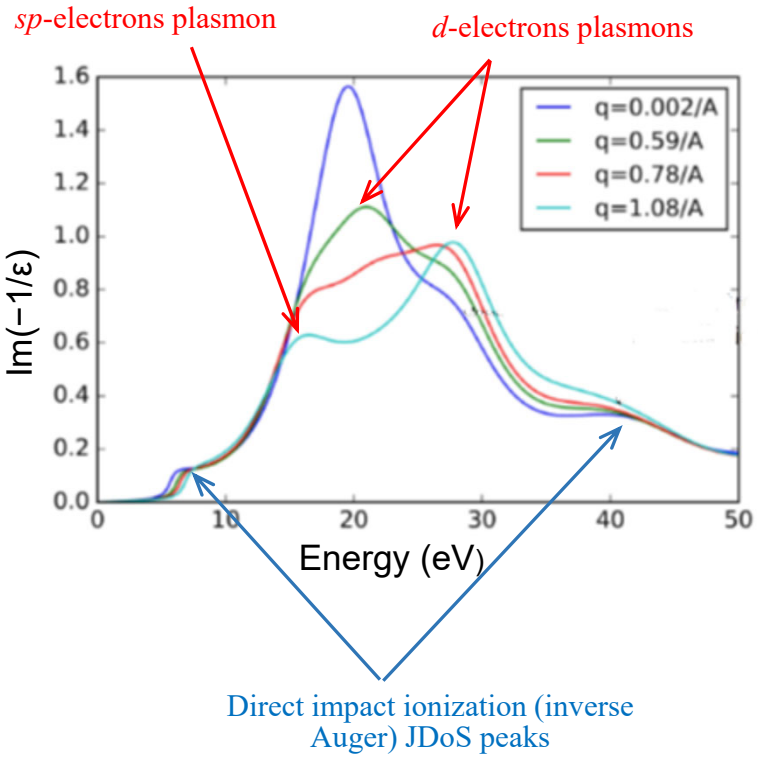
Experimental energy-loss spectra in $Al_xGa_{1-x}N$ (R. Dhall *et al.*, Appl. Phys. Lett. **112**, 061102 (2018), (quantum wells EELS, 60-300 keV)

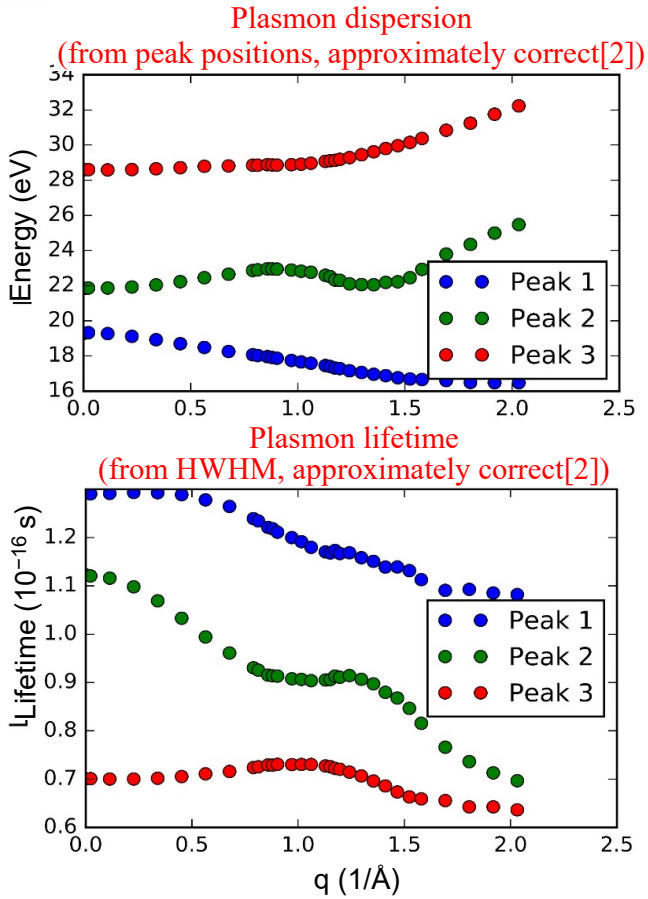


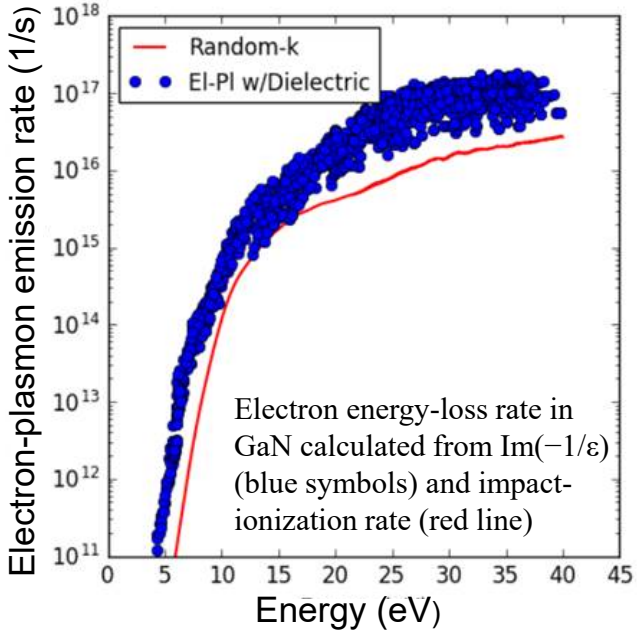
$$\epsilon^{(\mathrm{r})}(\mathbf{q},\omega) = 1 - \frac{e^2}{q^2\epsilon_0}\sum_{\mathbf{G},\mathbf{k},\mu,\mu'} \frac{[p(\mathbf{k},\mu)-p(\mathbf{k}+\mathbf{q},\mu')]\,|\langle \mathbf{k}+\mathbf{q}+\mathbf{G},\mu'|e^{i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k},\mu\rangle|^2}{E_\mu(\mathbf{k}) - E_{\mu'}(\mathbf{k}+\mathbf{q}) + \hbar\omega + i\hbar s}$$

(*Except for 'vertex corrections')

sp- and *d*-electrons plasmon: Dispersion and lifetime (GaN) [1]



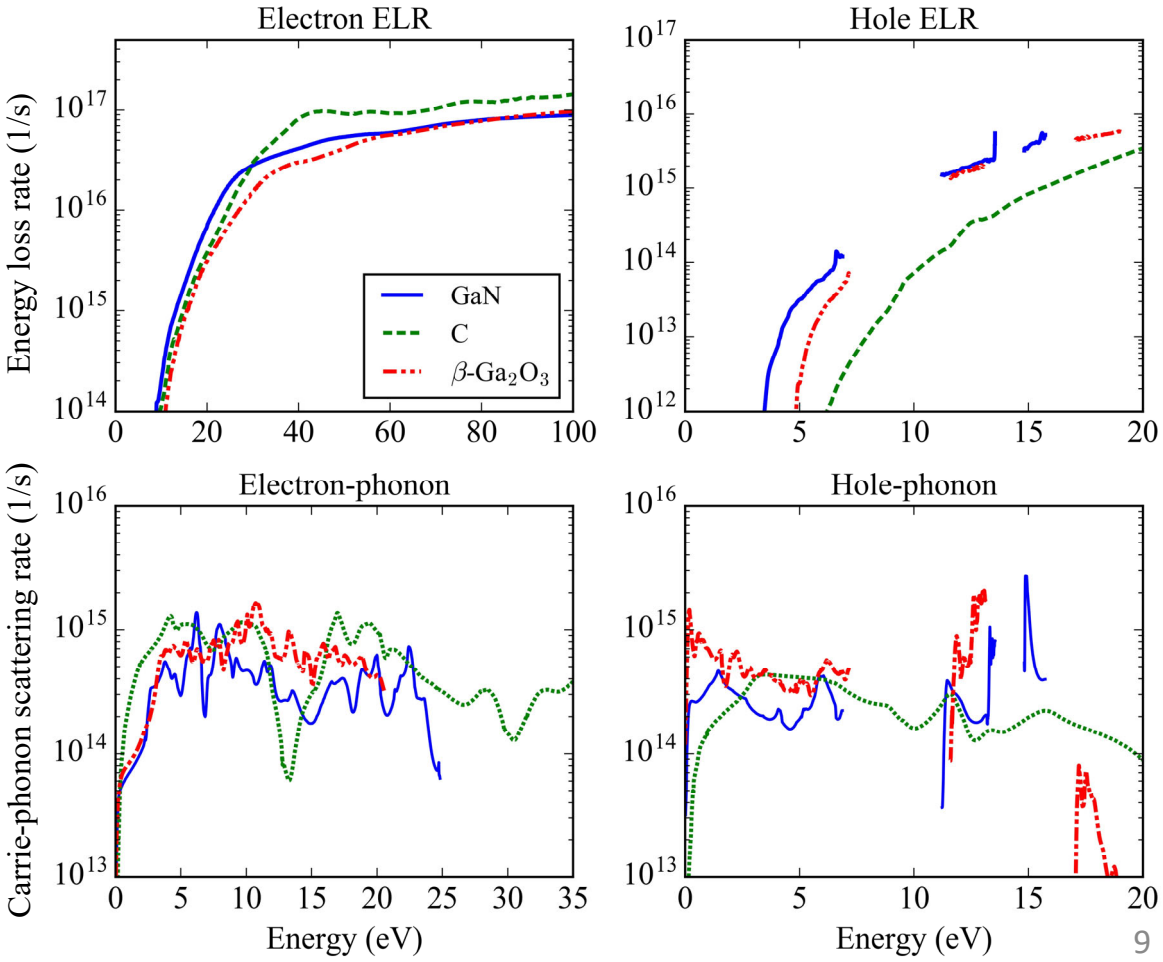




[1] D. O. Nielsen *et al.*, Phys. Rev. B **108**, 155203 (2023).
[2] P. Hamann *et al.*, Contrib. Plasma Phys. **10**, e202000147 (2020)

Scattering/Energy-Loss Rates

- Phonon scattering and ELR
- Electrons:
  - Phonon scattering dominant for low energies ($\lesssim$10-15 eV)
  - ELRs flatten as energy increases (reaches $\sim 10^{17}$ 1/s; broadening still acceptable)
  - Quinn, Ferrell, Pines, Penn calculated rates of similar magnitude [2-5]
  - Ga-based materials driven to high magnitudes by dense *d* bands; diamond by large loss function
- Holes:
  - Phonon scattering dominant for low energies
  - GaN spikes at ~13 and 15 eV from *d* bands



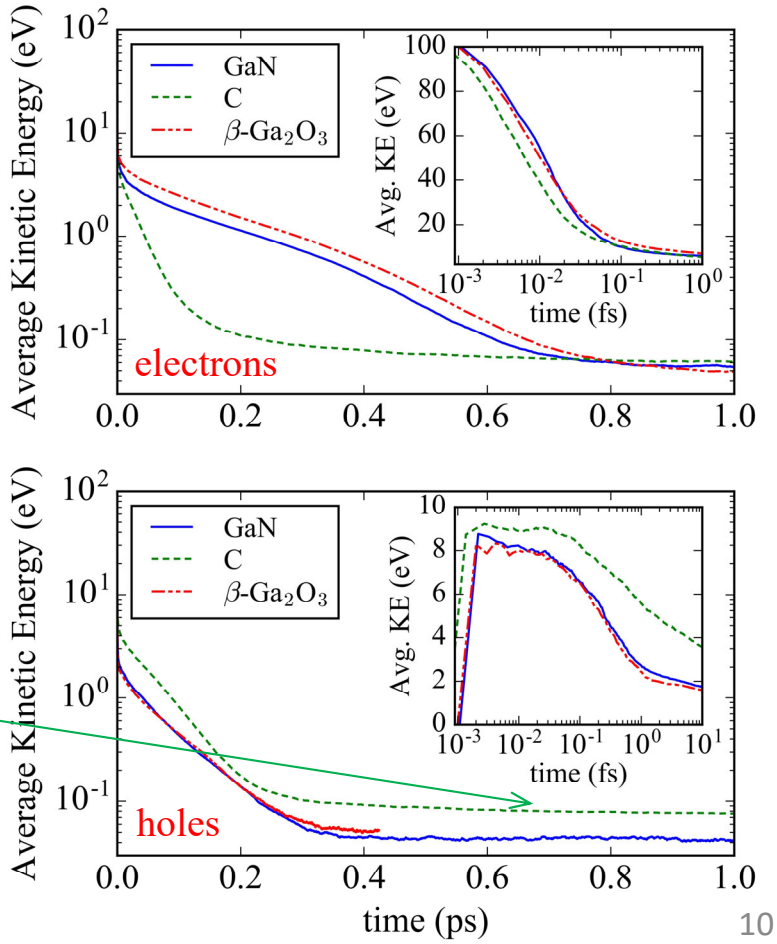
[1] D. O. Nielsen *et al*., Phys. Rev. B **108**, 155203 (2023) (GaN only).
[2] D. Pines, Rev. Mod. Phys. **28**, 184 (1956).
[3] J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1958).
[4] J. J. Quinn, Phys. Rev. **126**, 1453 (1962).
[5] D. R. Penn, Phys. Rev. **35**, 482 (1987).

Hot Electron Thermalization

- Solved semi-classical BTE
  - Full bands [1,2]
  - Zero field, 300 K
  - 1000 electrons ($E \sim 100$ eV)
- Electrons
  - Rapid energy loss ($t < 10^{-16}$ s)
  - Plasmon emission/impact ionization
  - Thermalization rate decreases ($t > 10^{-16}$ s)
  - Phonon scattering to thermal when energy falls below impact-ionization threshold
- Holes
  - Initial hole buildup
  - No rapid initial decrease (no plasma excitations)
  - Steeper slope (larger frame)

- GaN
  - Electrons thermalize in ~1 ps; holes in ~0.5 ps
  - Average energy per pair ~8.9 eV/pair [3,4]
- C (diamond)
  - Electrons thermalize in ~0.2 ps; holes in ~0.3 ps (large plasmons energy)
  - Average energy per pair ~12.87 eV/pair [5]
- β-Ga_2O_3
  - Electrons thermalize in ~1 ps; holes in ~0.5 ps
  - Average energy per pair ~11.24 eV/pair [4]

Slow hole thermalization in C due to small hole-phonon scattering rates below ~0.5 eV



[1] H. Shichijo and K. Hess, Phys. Rev. B **23**, 4197 (1981).
[2] M. V. Fischetti and S. E. Laux, Phys. Rev. B **38**, 14 (1988).
[3] P. J. Sellin and J. Vaitkas, Nucl. Instrum. Methods Phys. Res. A **557**, 479 (2006).
[4] E. B. Yakimov, *et al.*, Appl. Phys. Lett. **118**, 202106 (2021).
[5] J. W. Keister, *et al.*, J. Synchrotron Rad. **25**, 407 (2018).

New results

1. Thermalization of 100 eV electrons in Si and SiC
   - Small gap and Lorentzian broadening used by TurboEELs for ELF caused issues. Used "epsilon.x" instead.
2. Damage generated by hot electrons at the GaN-AlGaN interface of a HEMT stressed at high drain bias
   - Two defect precursors with small/slow observed V_{th}-shift (~10 mV/hour) [1]:

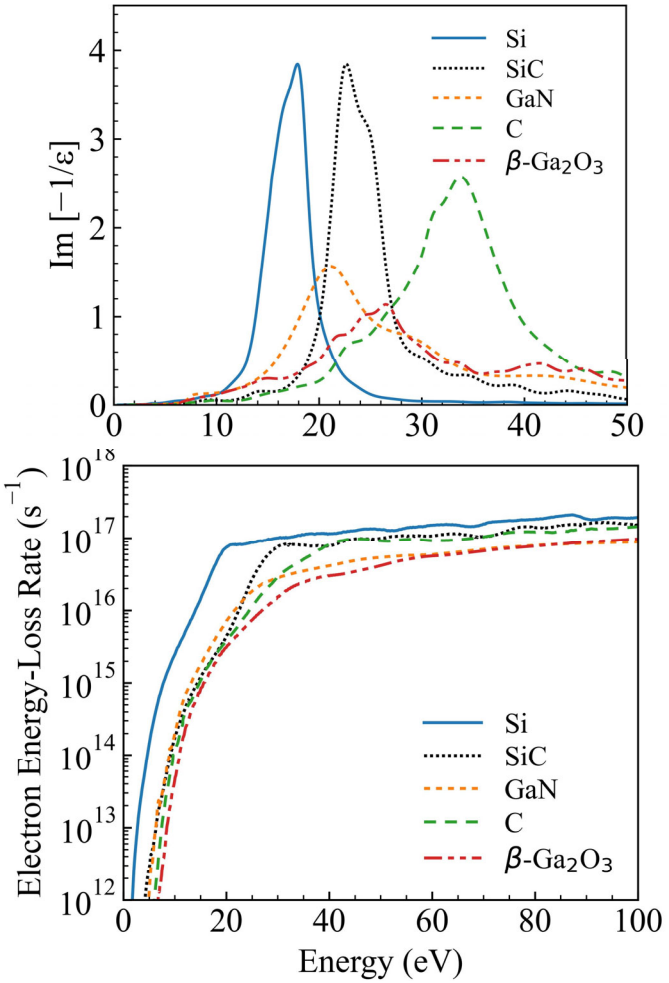
     $N_1^{\infty} = 1.46 \times 10^{11}$ cm^{-2} $\quad \sigma_1 = 8.2 \times 10^{-16}$ cm^2 $\quad E_1 = 0.6$ eV

     $N_2^{\infty} = 3.6 \times 10^{10}$ cm^{-2} $\quad \sigma_2 = 2.3 \times 10^{-16}$ cm^2 $\quad E_2 = 1.4$ eV
   - No GaN holes in Anduril (yet): Possible V_{th}-shift due to floating-body effects; faster/larger predicted V_{th}-shift (6 orders-of-magnitude): Increase E_1, E_2, decrease σ_1, σ_2)
3. Damage induced by 100 eV electrons in a GaN/AlGaN HEMT
   - No GaN holes in Anduril (yet): Only qualitative estimates for small density
4. Dehydrogenation of V_{Ga}-H_3 complexes at the GaN-AlGaN interface (p-channel HEMT)
   - Provided Laura and Sok hot-hole distributions to test their codes

[1] S. Mukherjee, Y. Puzyrev, J. Chen, D. M. Fleetwood, R. D. Schrimpf, and S. T. Pantelides, IEEE Trans. Electron Devices **63**, 1486 (2016)

1. Thermalization in Si and SiC

- Loss function of Si
  - Peak near predicted value (el gas: 16.4 eV)
  - Largest peak magnitude
- Loss function of SiC
  - Peak magnitude and area similar to Si
- Energy-loss rates
  - Si: reaches 10^{17} s^{-1} at ~20 eV; SiC: at ~30 eV
    - collisional broadening (~33 eV)
  - Caused by large loss function (peak magnitude and area)
  - Si: Small gap → large DOS for generated pairs
  - SiC: Large hole DOS → relatively large JDOS



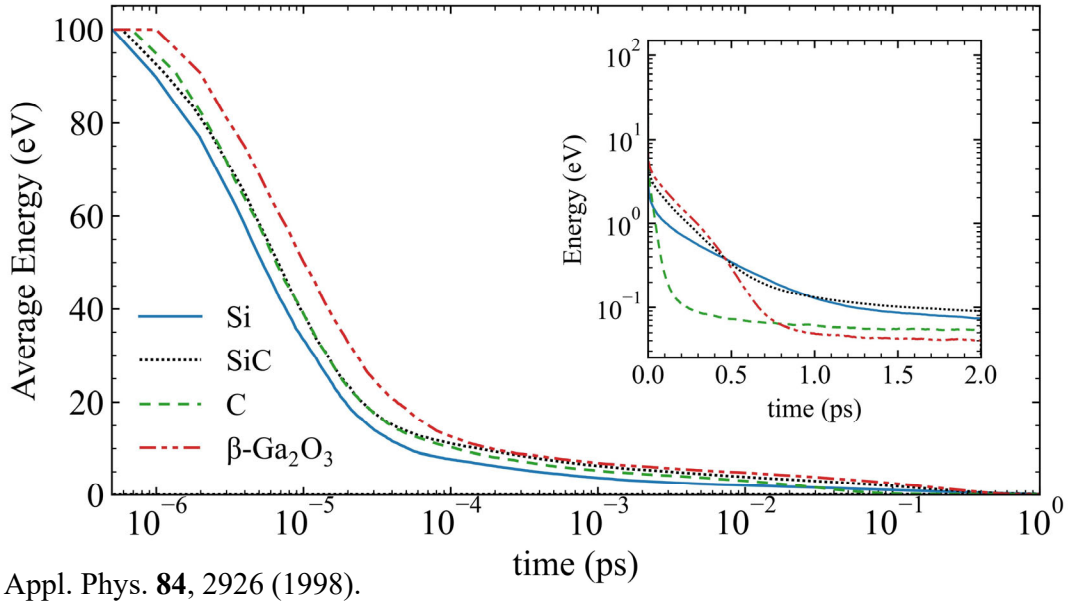
[1] D. O. Nielsen *et al*., Phys. Rev. B **108**, 155203 (2023) (GaN only).
[2] D. O. Nielsen and M. V. Fischetti, Appl. Phys. Lett. **123**, 252107 (2023) (Ga_2O_3 and C)

1. Thermalization in Si and SiC

- Initially, energy drops fastest in Si → high ELR
  - SiC and C nearly overlap → similar ELR
  - β-Ga_2O_3 lowest ELR (GaN very similar)
- Inset figure:
  - Final stages depend on phonon scattering rates
  - Low phonon scattering rates in Si and SiC cause slow thermalization.

- Pair creation energy:
  - Si: 3.4 eV/pair (Exp: 3.6 eV/pair [1])
  - SiC: 7.2 eV/pair (Klein's expression: 7.21 eV/pair [2])
  - GaN: 8.9 eV/pair
  - β-Ga_2O_3: 11.2 eV/pair
  - C: 12.9 eV/pair

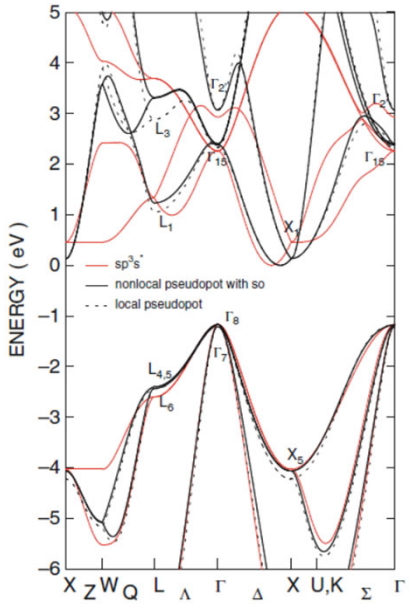
  (slide 10)

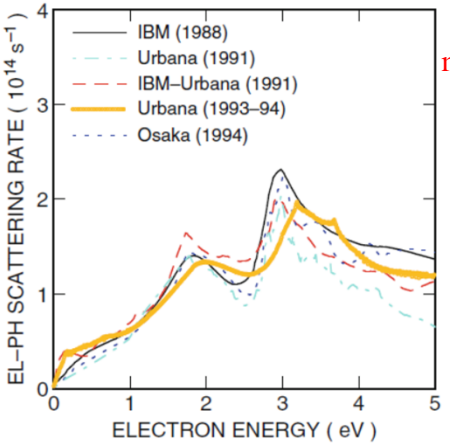


[1] F. Scholze, H. Rabus, and G. Ulm, J. Appl. Phys. **84**, 2926 (1998).
[2] C. A. Klein, J. Appl. Phys. **39**, 2029 (1968).

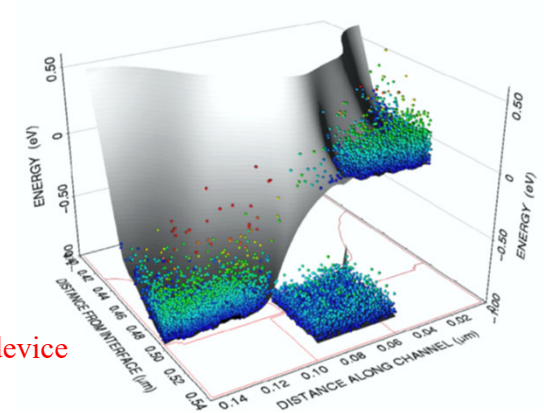
2. The template of much older work: Damage generated at the interface of a Si MOSFET

Empirical-pseudopotential/DFT band structure [1]



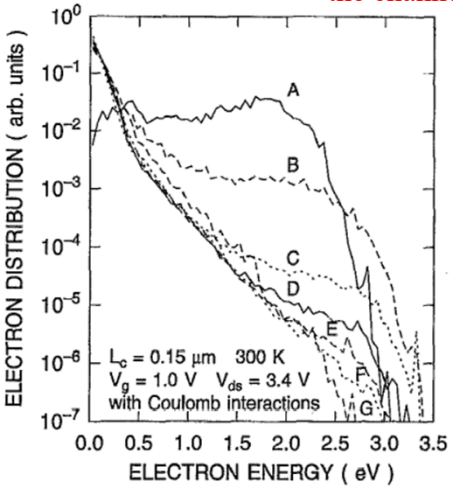


Electron-phonon (and more) scattering rates [1]

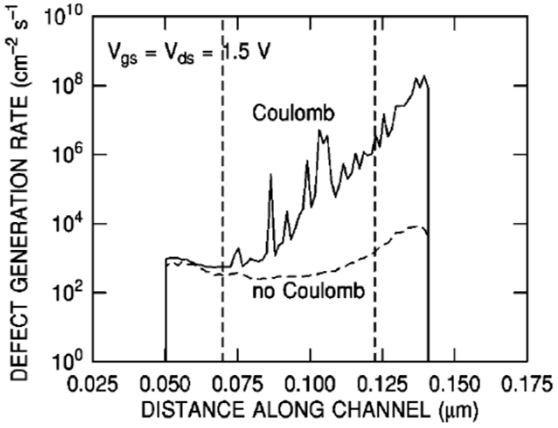


The device

Hot carriers along the channel [1]



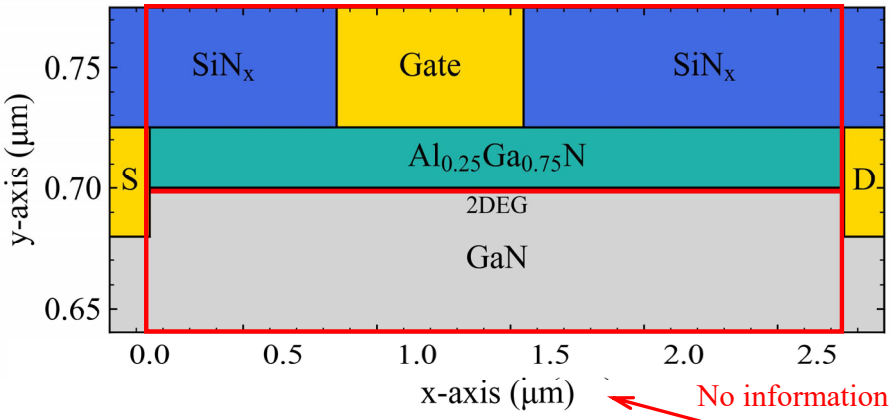
Defects generated at the Si/SiO_2 interface: $P_g = \exp(E/\Delta E)$ (empirical model) [2]



[1] M. V. Fischetti, S. E. Laux, and E. Crabbé, J. Appl. Phys. **78**, 1058 (1995); M. V. Fischetti and S. E. Laux, J. Appl. Phys. **89**, 1205 (2001); [2] D. J. DiMaria, J. Appl. Phys. **87**, 8707 (2000)

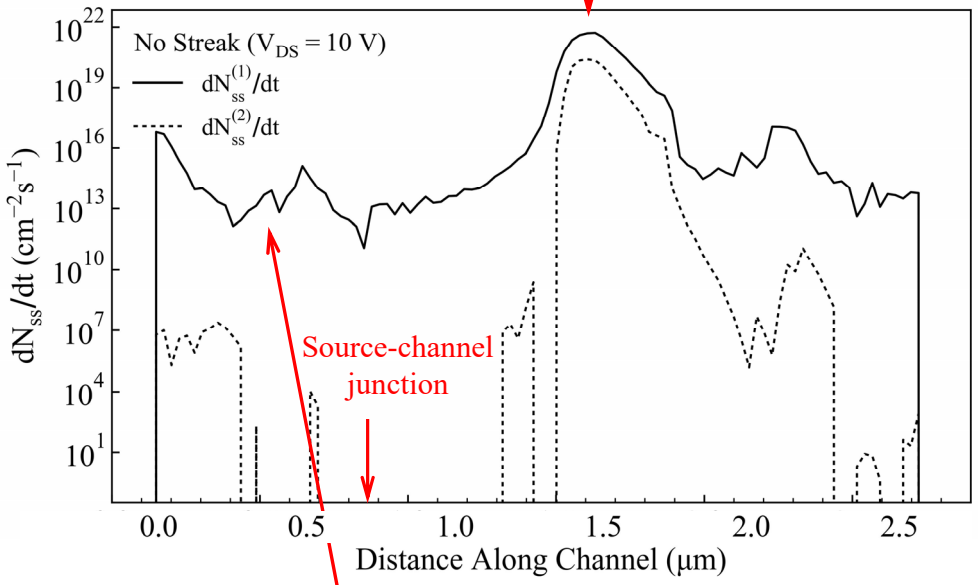
2. Damage generated at the GaN-AlGaN interface of a HEMT

- Hot-electron induced damage at the GaN-AlGaN interface of n-channel HEMTs [1]
- With published parameters (N_∞, σ_i), found very high defect-generation rate near the source, ~10^{13} $cm^{-2}s^{-1}$ @ V_{DS}=10 V; but: very slow V_{th} shift (~10 mV/hours), seen in experiments, ~10^{6} $cm^{-2}s^{-1}$ @ V_{DS}=20 V [1]



No information about SiC body contact. Crucial to assess role of holes (floating body?, parasitic bipolar?)

Mid-channel and drain-end: Precursor defects ($1.8x10^{11}$ cm^{-2}) generated almost instantly (in ~10 ps)

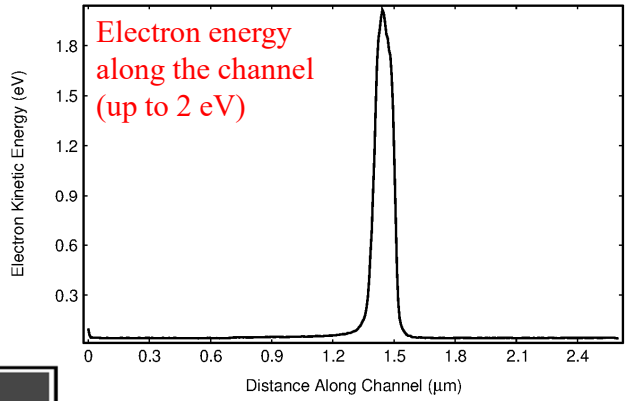


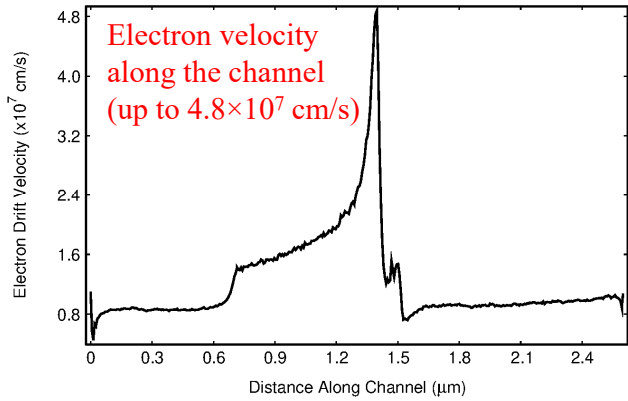
Source-end: High defect generation rate, inconsistent with experiments

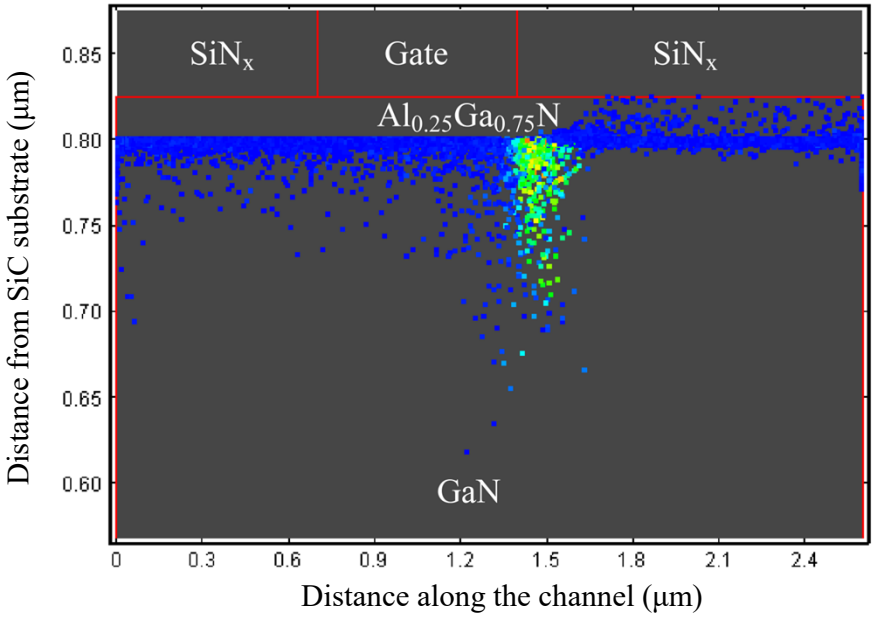
[1] S. Mukherjee, Y. Puzyrev, J. Chen, D. M. Fleetwood, R. D. Schrimpf, and S. T. Pantelides, IEEE Trans. Electron Devices **63**, 1486 (2016)

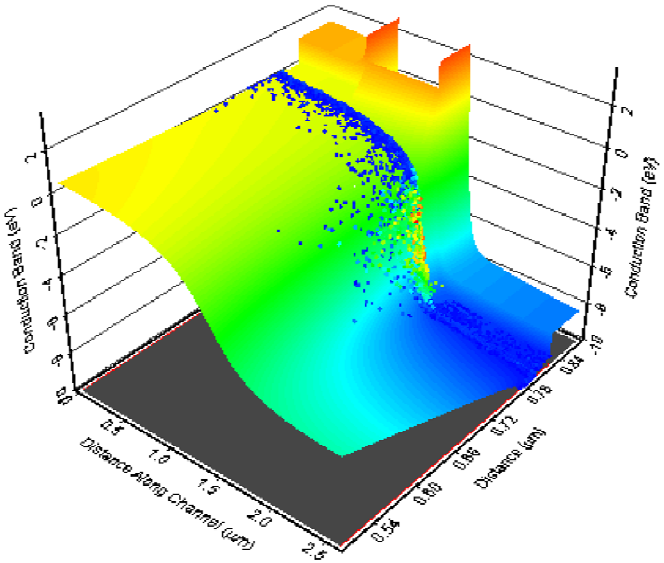
2. Damage generated at the GaN-AlGaN interface of a HEMT

- GaN-AlGaN n-channel HEMT; V_{DS} = 10 V, V_{GS} = 0 V
- Hot electrons near drain-edge of gate →
  Large defect generation rate near drain
- Mostly thermal electrons near source →
  Small defect generation rates



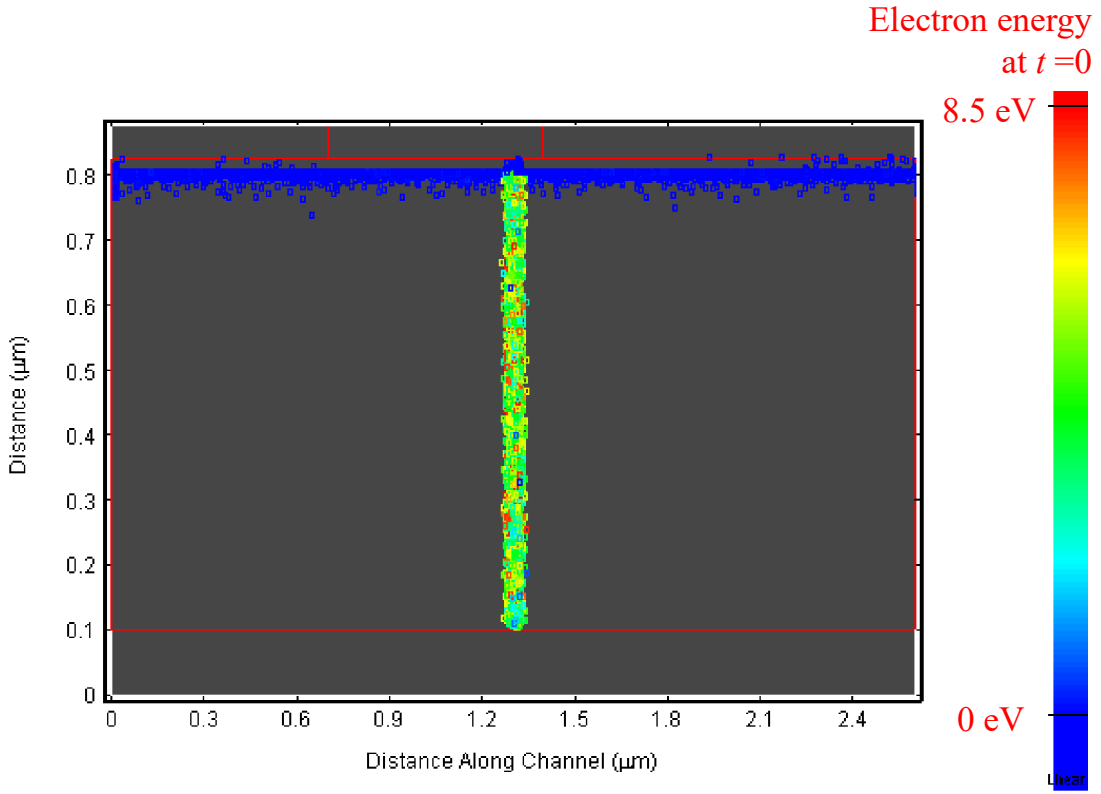






3. Damage induced by 100 eV electrons in a GaN/AlGaN HEMT

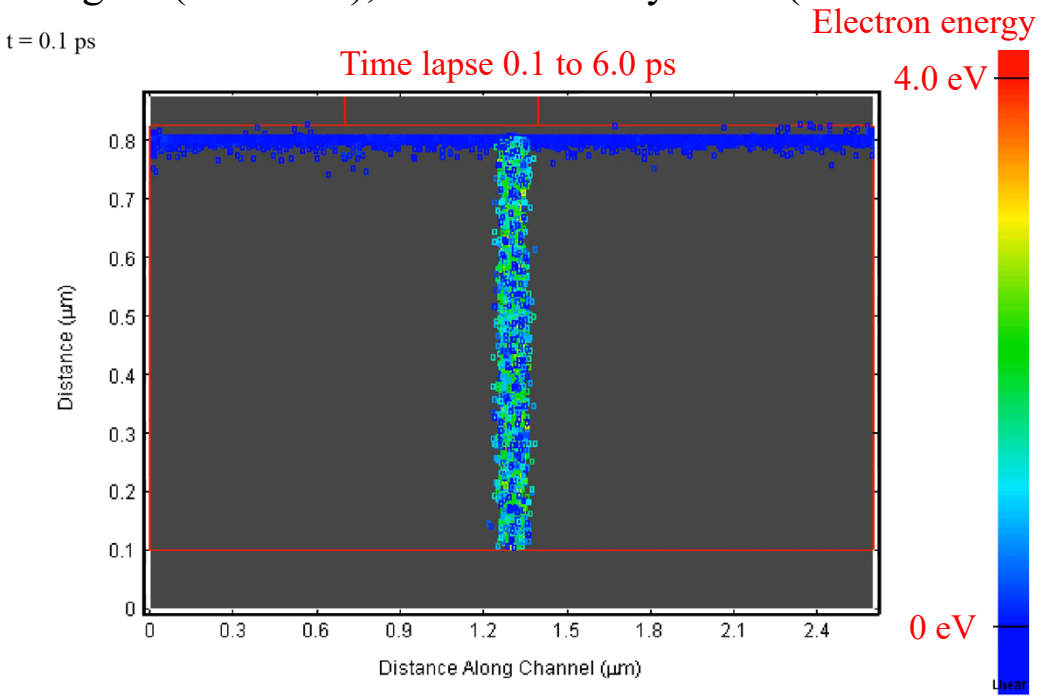
- Mimic with optically-generated pairs ($h\nu = 12.1$ eV) the spatial and energetic pair distribution from 100 eV relaxation after 120 fs:
  - Average electron energy ~8.7 eV
  - Gaussian width ~20 nm
  - Initial peak density ~10^{18} cm^{-3}, (expect 10^{21}-10^{22} cm^{-3}, for a 10 MeV proton [1], LET~10-15 MeV cm^2/mg ~6×10^{10} eV/cm)
- Calculate generation rate of defects at the GaN-AlGaN interface of an n-channel HEMT at V_{DS} = 1 V



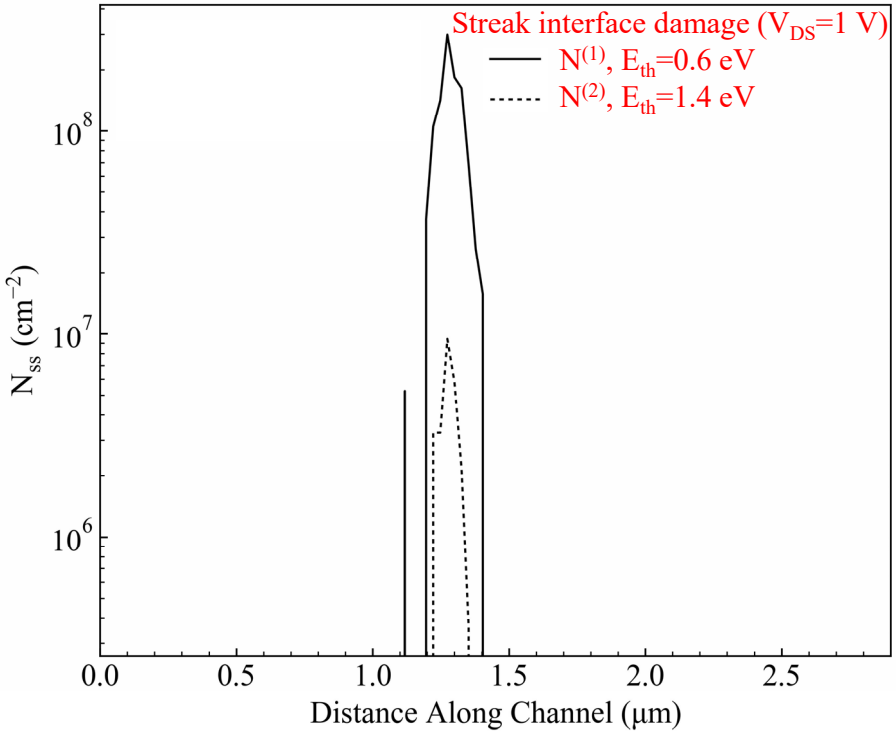
[1] J. Osheroff *et al*., IEEE Trans. Nucl. Sci**. 68**, 597 (20121).

3. Damage induced by 100 eV electrons in a GaN/AlGaN HEMT

- Low V_{DS} (1 V) prevents damage from energetic electrons in channel
- Damage from streak confined to relatively narrow region (~300 nm); induced at early times (<1 ps)



Peak 'streak' density 10^{18} cm^{-2}, Gaussian width ~20 nm

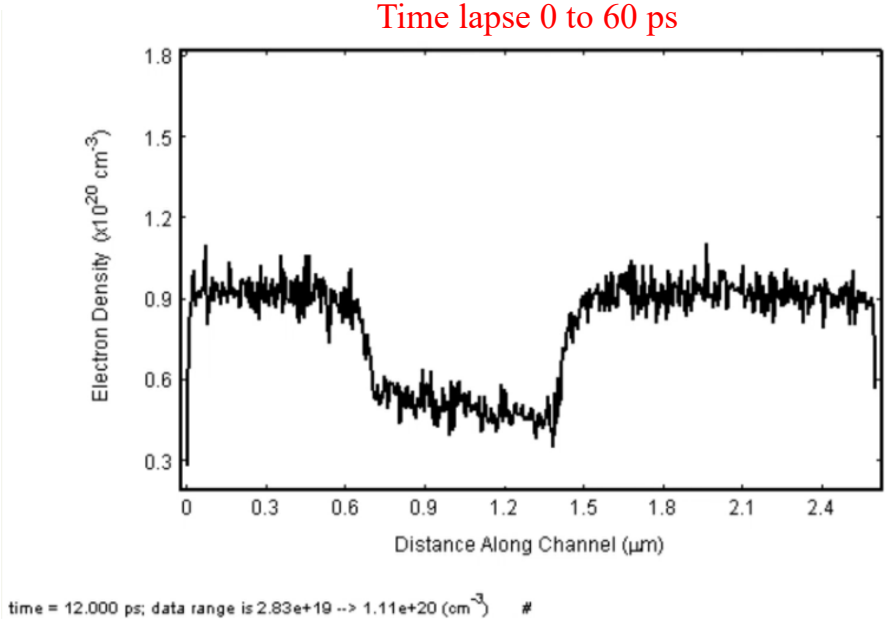


Issues: 1. Frozen field (no holes)
2. Zero total momentum (need info from Geant4)
… but likely already isotropic in ~100 fs)

3. Damage induced by 100 eV electrons in a GaN/AlGaN HEMT

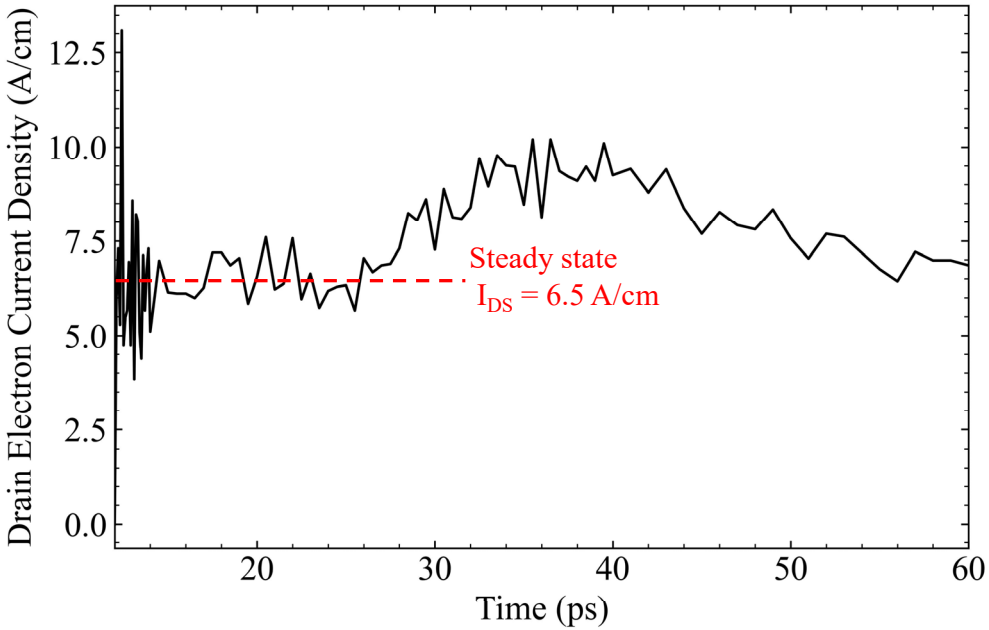
- Track radiation-induced excess charge and current at the contacts
- Video: Carrier density in channel as function of time
  - "Wave" of electrons builds near streak location
  - Moves toward drain contact and disappears after ~ 40 ps

Electron density along channel
Time lapse 0 to 60 ps



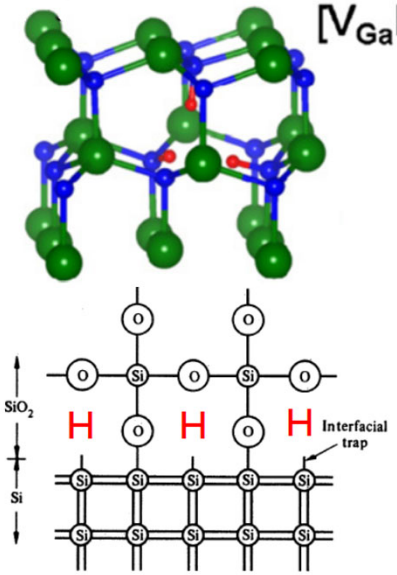
- This behavior is reflected in plot of current vs. time
  - Initially, current density remains near pre-streak levels
  - Apparent increase in current at about 25 ps signifies arrival of "wave"

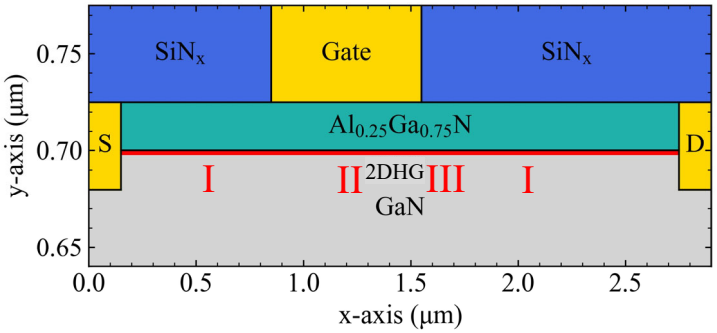
Displacement current not available (frozen field).
Need holes and self-consistency with Poisson (Ramos theorem).

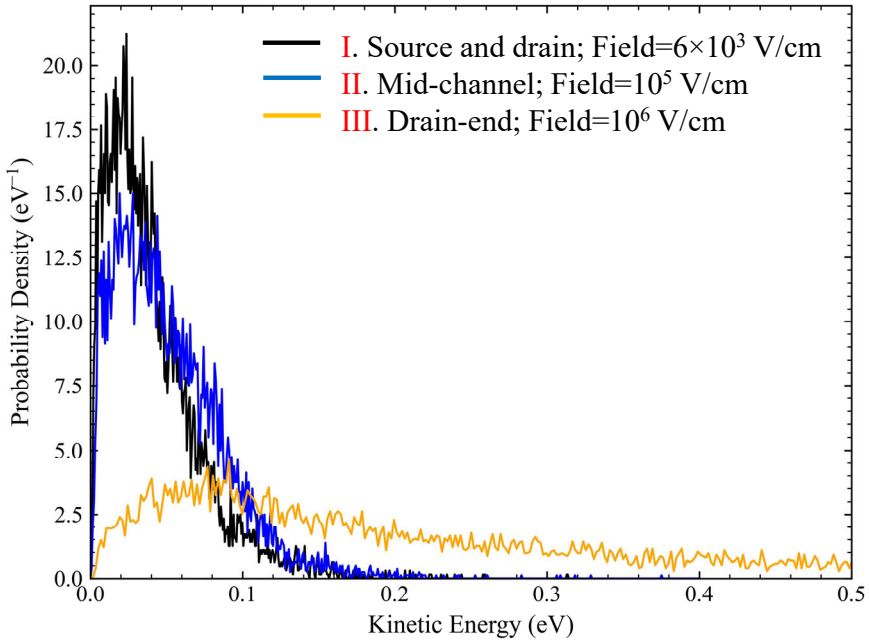


4. Dehydrogenation of V_{Ga}-H_3 complexes at the GaN-AlGaN interface

- Study of the dehydrogenation of V_{Ga}-H_3 complexes at the GaN-AlGaN interface [1,2] of a p-channel HEMT. Holes are easier: higher DoS – Nichols, Pantelides (VU), and Zhang (UF)
- Monte Carlo hole energy distributions in GaN serve as input to calculate dehydrogenation rate
- …in progress







[1] S. T. Pantelides *et al.*, Microelectron. Eng. **90**, 3 (2012)
[2] L. Nichols, unpublished and PhD Thesis (2024)

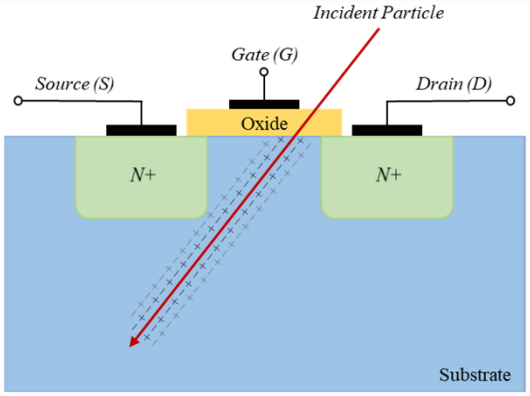
Conclusions and plans

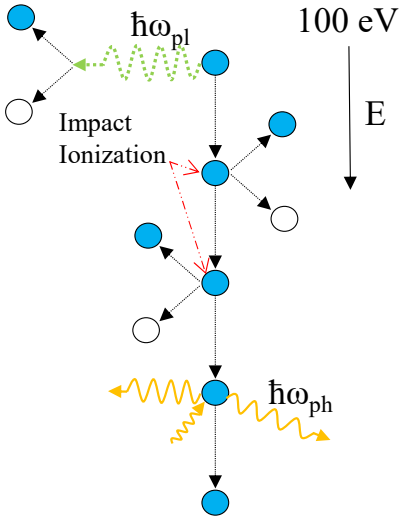
- First principles study of electron transport in the "10-100 eV gap" (wurtzite GaN, C-diamond, β-Ga_2O_3, Si, SiC)
  - Included band structure effects up to 100 eV
  - Studied plasmon and impact ionization in this regime
    - Very short plasmon lifetime
    - Fast ($10^{-17} - 10^{-16}$ s) plasmon-induced energy losses; phonon-assisted thermalization in 1 ps or so
    - Spatial 'spread' of ~ 100-200 nm in the first ps (bad for devices?), highly anisotropic in β-Ga_2O_3
    - Average energy/pair ($\lesssim 2 - 3E_{gap}$) in agreement with experimental values
- Ready (almost) to study SEEs/SEUs and radiation-induced device degradation
    - Studied relaxation of the 'streak' in GaN/AlGaN HEMTs, but must implement MC holes
    - Calculation of transport characteristics of C, β-Ga_2O_3, … (low-field mobility, velocity-field)
    - Collaborate with Vanderbilt Univ. (Fleetwood, Pantelides, Schrimpf) to account for hot-electron defect generation (*e.g.*, H release) and for scattering with radiation-induced defects in FETs
  - Study carrier relaxation in other materials (SiO_2, AlN, AlGaN, etc.)
  - Investigate temperature effects (?)

More stuff

Overview of the problem

- Ionizing radiation in devices → high-energy charge carriers
  - Nuclear/particle physics community: Binary-collision codes [1,2]
    - Accurate down to ~ 100 eV [3]
    - Band structure effects?
  - Electronic device community: Full-band Monte Carlo [4]
    - Region below ~ 5-10 eV: well studied
  - Intermediate energy range: ~ 10-100 eV
    - Energy-loss processes: free-electrons, plasmon emission -- mostly MFP in metals [5], simplified models in semiconductors [6,7] and SiO_2 [8], no phonon losses, no time scale of the dynamics
- Close the 'gap' using *ab initio* methods
- Increasing interest in wide-bandgap materials
  - Focus on GaN (wurtzite), C (diamond), and β-Ga_2O_3





"Hic Sunt Dracones"
"Here be dragons"

[1] R. A. Reed, *et al.*, IEEE Trans. Nucl. Sci. **62**, 1441 (2015).
[2] S. Agostinelli, *et al.*, Nucl. Instrum. Methods Phys. Res. A: Accel. Spectrom. Detect. Assoc. Equip. **506**, 250 (2003).
[3] C. M. Dozier and D. B. Brown, IEEE Trans. Nucl. Sci. **28**, 4137 (1981).
[4] H. Shichijo and K. Hess, Phys. Rev. B **23**, 4197 (1981).
[5] D. Pines, Rev. Mod. Phys. **28**, 184 (1956). J. J. Quin and R. A. Ferrel, Phys. Rev. **112**, 812 (1958); J. J. Quinn, Phys. Rev. **126**, 1453 (1962); D. R. Penn, Phys. Rev B. **35**, 482 (1982).
[6] R. C. Alig, S. Bloom, and C. W. Struck, Phys. Rev. B **22**, 5565 (1980).
[7] A. Akkerman, J. Barak, and D. Emfietzoglou, Nucl. Inst. Meth. Phys. Res. B **227,** 319 (2005).
[8] G. A. Ausman Jr. and F. B. McLean, Appl. Phys. Lett. **26**, 173 (1975).

Scattering rates from the energy-loss function: Numerical details

- Discretize the Brillouin zone (as usual) into volume elements centered at $\mathbf{k}_j$ with density of states $\mathcal{D}_{jn}(E)$ for band n at energy E (from the Gilat-Raubenheimer [1] or tetrahedron [2] methods); tabulate $E_n(\mathbf{k}_i)$
- Discretize the ω-axis into elements of width $\Delta\omega$ centered at ω_r and tabulate $\mathrm{Im}\left[\frac{-1}{\varepsilon(\mathbf{q}_i,\omega_r)}\right]$
- Evaluate energy-loss rate:

Replaced by $|\mathbf{q}_i|$ (isotropic)

as:

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

$$\frac{1}{\tau_n(\mathbf{k}_i)} = 2\pi e^2 \sum_{n',\omega_r} \Delta\omega \sum_{\mathbf{k}_j} \frac{1}{|\mathbf{k}_i - \mathbf{k}_j|^2} \mathrm{Im}\left[\frac{-1}{\varepsilon(|\mathbf{k}_i - \mathbf{k}_j|, \omega_r)}\right] \mathcal{D}_{jn'}[E_n(\mathbf{k}_i) - \hbar\omega_r].$$

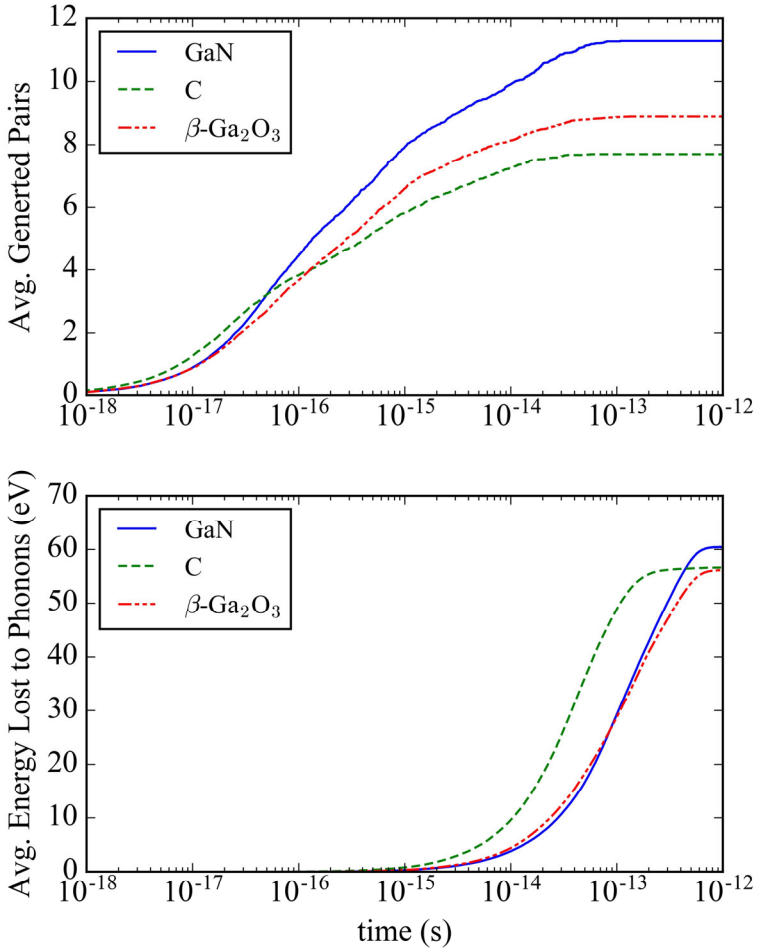
The sum over $\mathbf{k}_j$ spans only 'energy-conserving' elements selected using the Gilat-Raubenheimer [1] or Blöchl's tetrahedron method [2]

- In the Monte Carlo simulations, after a collision, select a random band n', wavevector $\mathbf{k}_j$, and energy-loss $\hbar\omega_r$ with probability distribution given by the 'integrand' of the equation above (using the 'rejection technique'[3])
- Account for Landau damping by generating an electron-hole pair with total kinetic energy $\hbar\omega_r - E_{\mathrm{gap}}$

[1] G. Gilat and L. J. Raubenheimer. Phys. Rev. **144**, 390 (1966).
[2] P. E. Blöchl, O. Jepsen, and O. K. Andersen, Phys. Rev. B **49**, 16223 (1994).
[3] Jacoboni and L. Reggiani, Rev. Mod. Phys. **55**, 645 (1983).

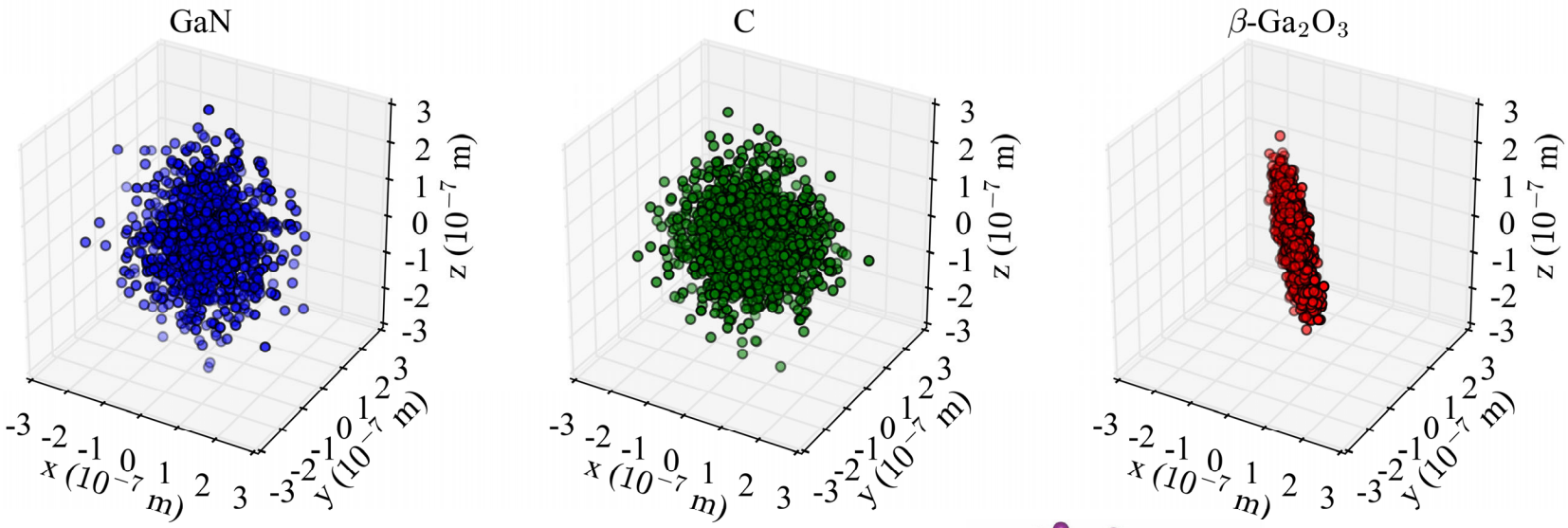
Where does the energy go?

- At short times, for $t < 10^{-14}$ s, energy distributed among e-h pairs
- At $\sim 10^{-14}$ s, phonon emission increases significantly, pair generation flattens
- Somewhat more energy deposited into lattice for GaN than C and Ga_2O_3 (60% *vs*. 56-57%) .
- Fewer pairs generated in C and Ga_2O_3
  → larger creation energy
- Left-over energy: Recombination [1], ignored here (small density for Auger, much longer times for SRH)
- Temperature effects
  - Ignore, for now: Assume low carrier/phonon density
  - No problems early on, may be a factor for $t > 10^{-13}$ s

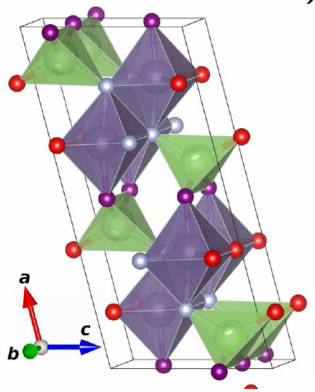


[1] S. Jursenas, *et al.*, J. Cryst. Growth **281**, 161 (2005).

Diffusion in real space



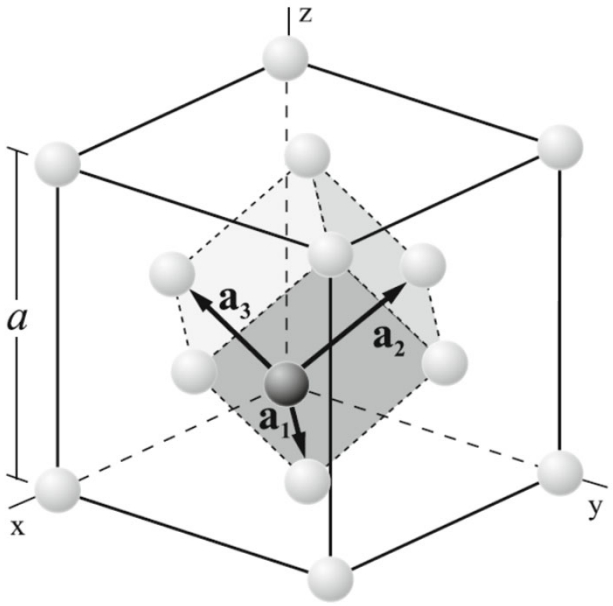
- After full thermalization, ~1 ps , electrons diffuse over ~ 100 nm
  - Approximately isotropic in C and GaN, strongly anisotropic in β-Ga_2O_3 (following long edge of unit cell)



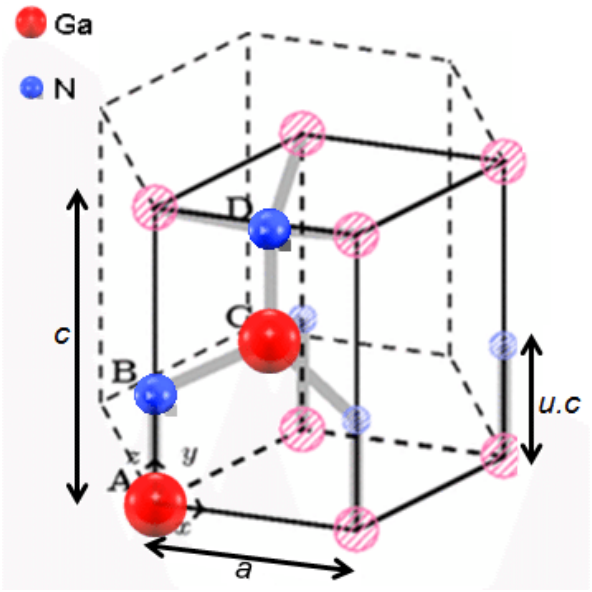
Unit cell of β-Ga_2O_3

H. Peelaers and C. Van de Walle, Phys. Stat. Sol. B **252**, 828 (2015) .

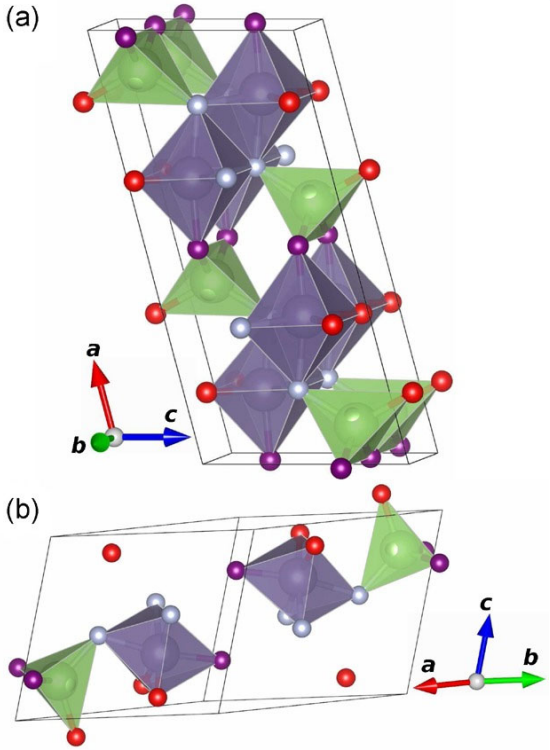
Wigner-Seitz cells:
C (diamond), GaN (wurtzite), β-Ga_2O_3



C (diamond, Fd3m)
fcc, 2 atoms/WS cell [1]



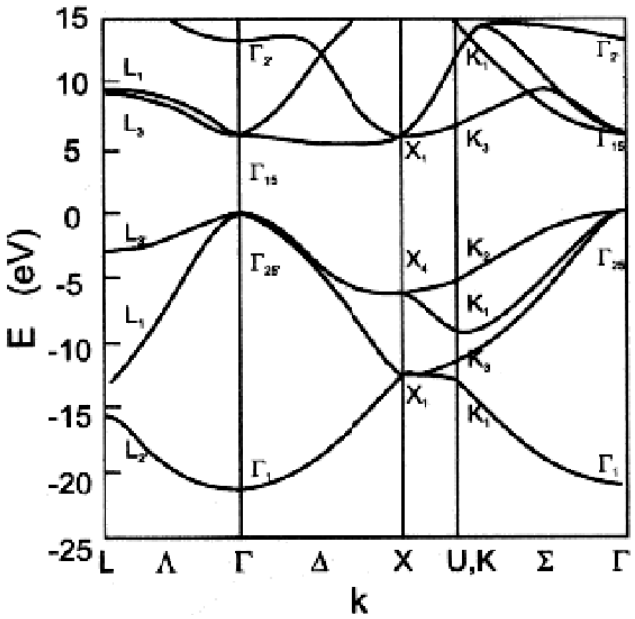
GaN ($P6_3mc$)
wurtzite, 4 atoms/WS cell [2]



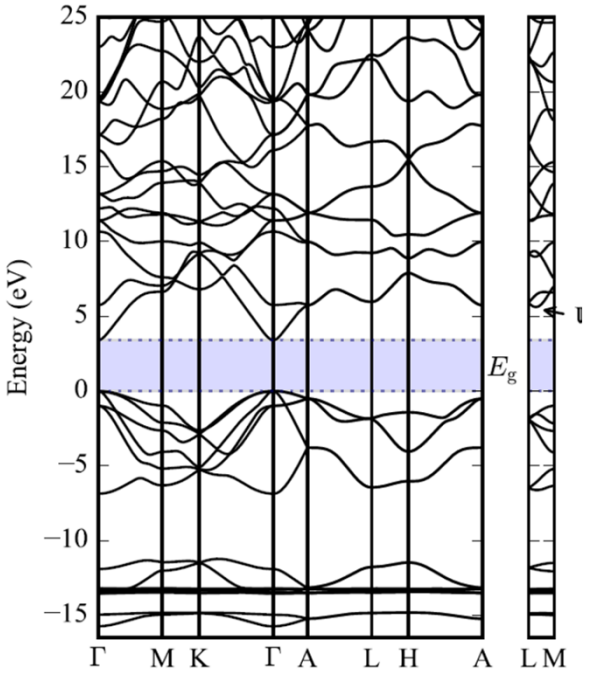
β-Ga_2O_3 (C2/m)
monoclinic, 10 atoms/WS cell [3]

[1] M. V. Fischetti and W. V. Vandenberghe, *Advanced Physics of Electron Transport in Semiconductors and Nanostructures* (Springer, 2016)
[2] D. Andiwijayakusuma *et al*.,J. Phys.: Conf. Ser. **739**, 012027 (2016).
[3] H. Peelaers and C. Van de Walle, Phys. Stat. Sol. B **252**, 828 (2015) .

Band structure:
C (diamond), GaN (wurtzite), β-Ga_2O_3

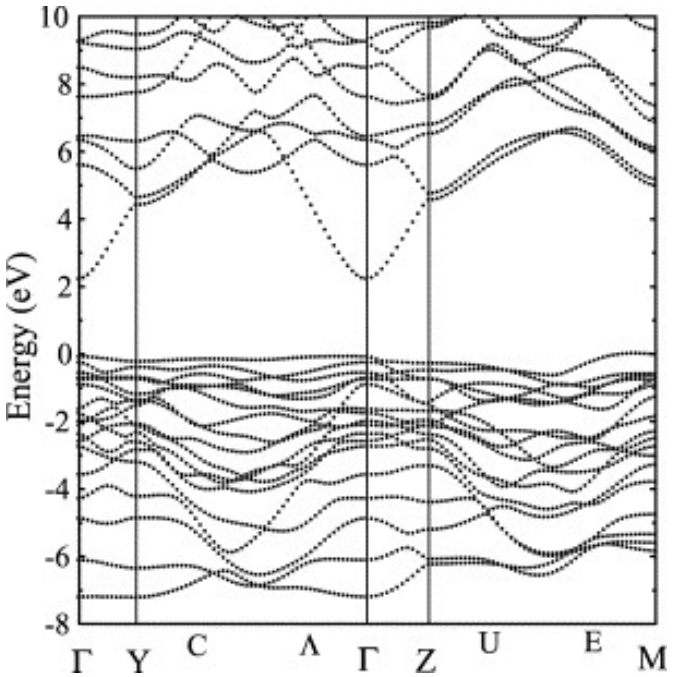


C (diamond, HSE-ONCV) [1]
PBESOL-USSP for 'el-ph & $\varepsilon(q,\omega)$
$E_{\mathrm{gap}} = 5.45$ eV



GaN (PBE-ONCV) [2]

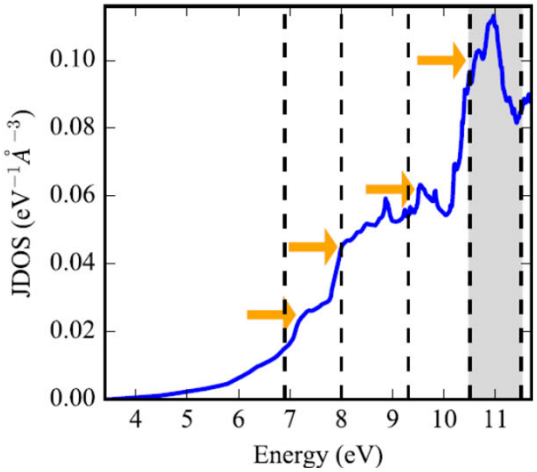
$E_{\mathrm{gap}} = 1.78$ eV $\rightarrow 3.4$ eV



β-Ga_2O_3 (PBE-ONCV) [3]
PBESOL-USSP for 'el-ph & $\varepsilon(q,\omega)$
$E_{\mathrm{gap}} = 2.63$ eV $\rightarrow 4.8$ eV

[1] M. Dipalo, *Nanocrystalline diamond growth and device applications,* (Doctoral Thesis, Ulm University, 2008)
[2] D. O. Nielsen *et al*., Phys. Rev. B **108**, 155203 (2023).
[3] K. Yamaguchi, Solid State Commun. **131**, 739 (2004) .

Can we trust DFT up to 100 eV? The case of GaN



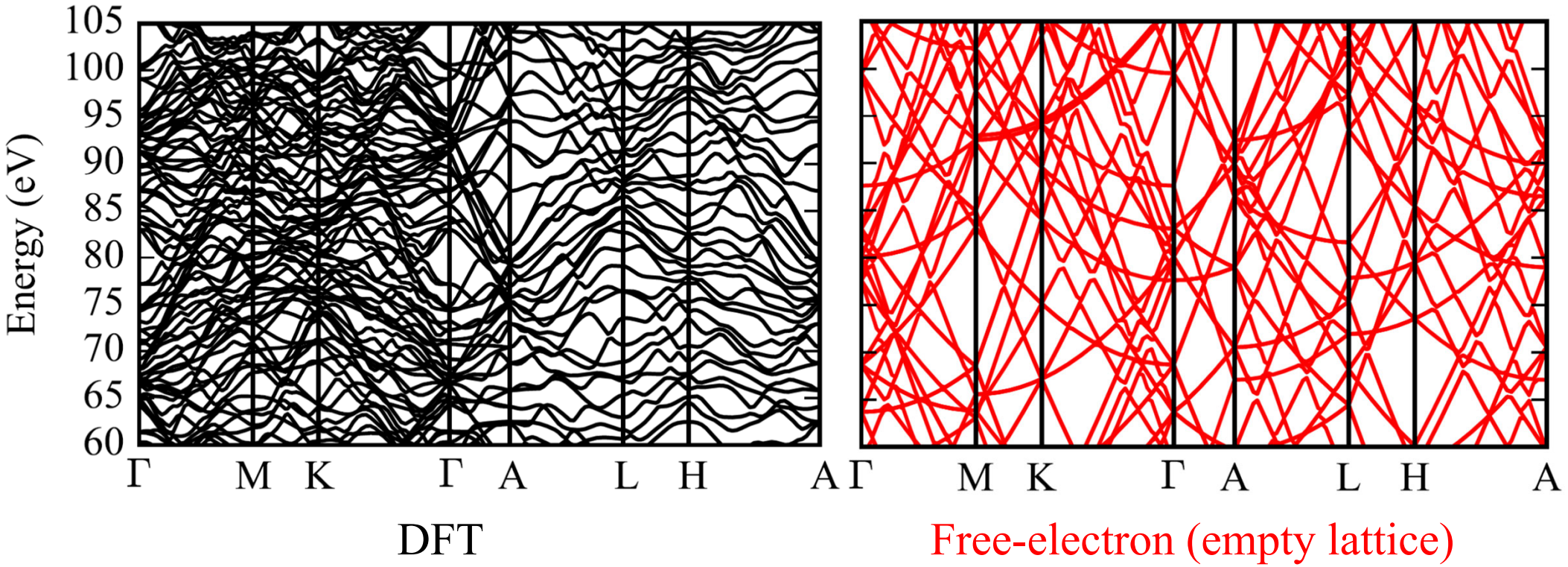
DFT-calculated JDOS *vs*. *E* of GaN [1]
Dashed lines: Vertical transition energies [2]
Orange arrows: JDOS peaks and

So: OK up to ~10 eV
More and more free-electron-like at higher energies?

	$U_{v_1-c_1}$	$M_{v_1-c_2}$	$L_{v_1-c_1}$	$K_{v_1-c_1}$	$K_{v_2-c_1}$	$A_{v_1-c_3}$	$L_{v_3-c_3}$
Our work (GGA-PBE) [1]	7.18	8.00	7.80	9.42	9.68	10.49	11.10
DFT-LDA [2]	6.87	7.65	7.64	9.57	9.68	10.53	11.05
Exp. [2]	6.9	8.0	8.0	9.3	9.3	10.5–11.5	10.5–11.5
Exp. [3]	7.1	8.1	8.1	9.2	9.2		
Exp [4]	7.0	7.9	7.9	9.0	9.0		

[1]] D. O. Nielsen *et al*., Phys. Rev. B **108**, 155203 (2023).
[2] W. R. L. Lambrecht *et al*., Phys. Rev. B **51**, 13516 (1995).
[3] G. Brockt and H. Lakner, Micron **31**, 435 (2000).
[4] S. Logothetidis *et al*., Phys. Rev. B **50**, 18017 (1994).

Free electrons at 100 eV? Hm…



DFT

Free-electron (empty lattice)

D. O. Nielsen *et al.*, Phys. Rev. B **108**, 155203 (2023).

Can we use 1st–order perturbation theory?

- Scattering rates as high as $5 \times 10^{16} - 10^{17}$/s for 100 eV electrons imply a broadening $\Delta E \sim \hbar/\tau \sim$30-60 eV
  - Problem discussed by Quinn [1]: "[…] *the quasiparticle concept is not too bad*"
  - Concerns even worse at lower energy (~5 eV): The Capasso-Hess controversy of the '80s [2,3]: For impact ionization in GaAs, $\Delta E \gtrsim E$!
  - The 'solution' (*i.e.*, collisional broadening') worse than the original problem: 2nd –order corrections 'corrected' by higher-order terms
  - Bethe-Salpeter equation (Coulomb e-h interaction, matters in low-ε materials) does not help (→probably even higher rates). Need full quantum transport model (NEGF+DFT), unrealistic with up to 350 bands

From J. J. Quinn, Phys. Rev. **126**, 1453 (1962) (metals, free-electron model, Lindhard)

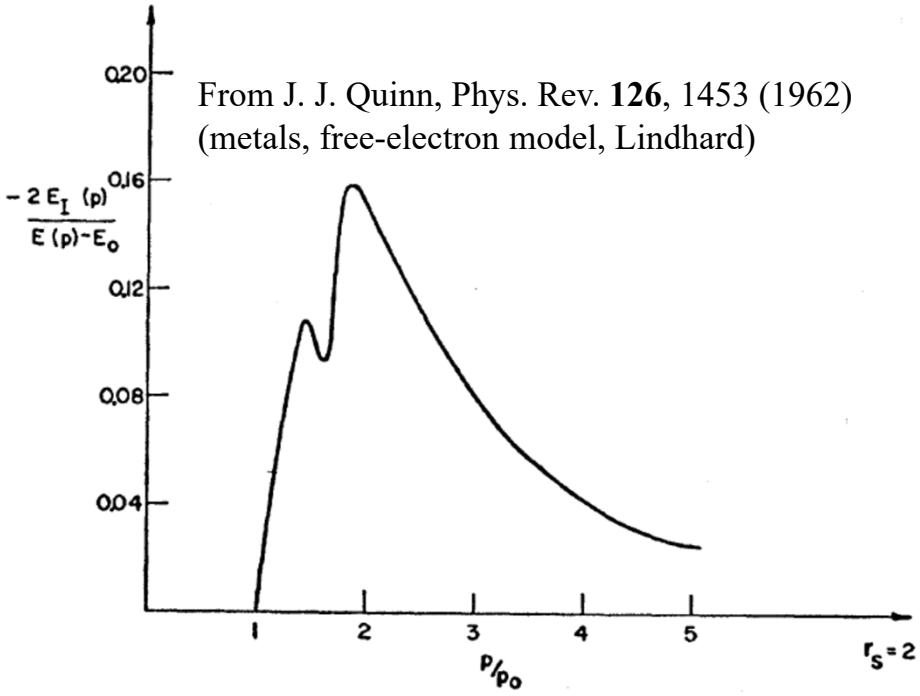
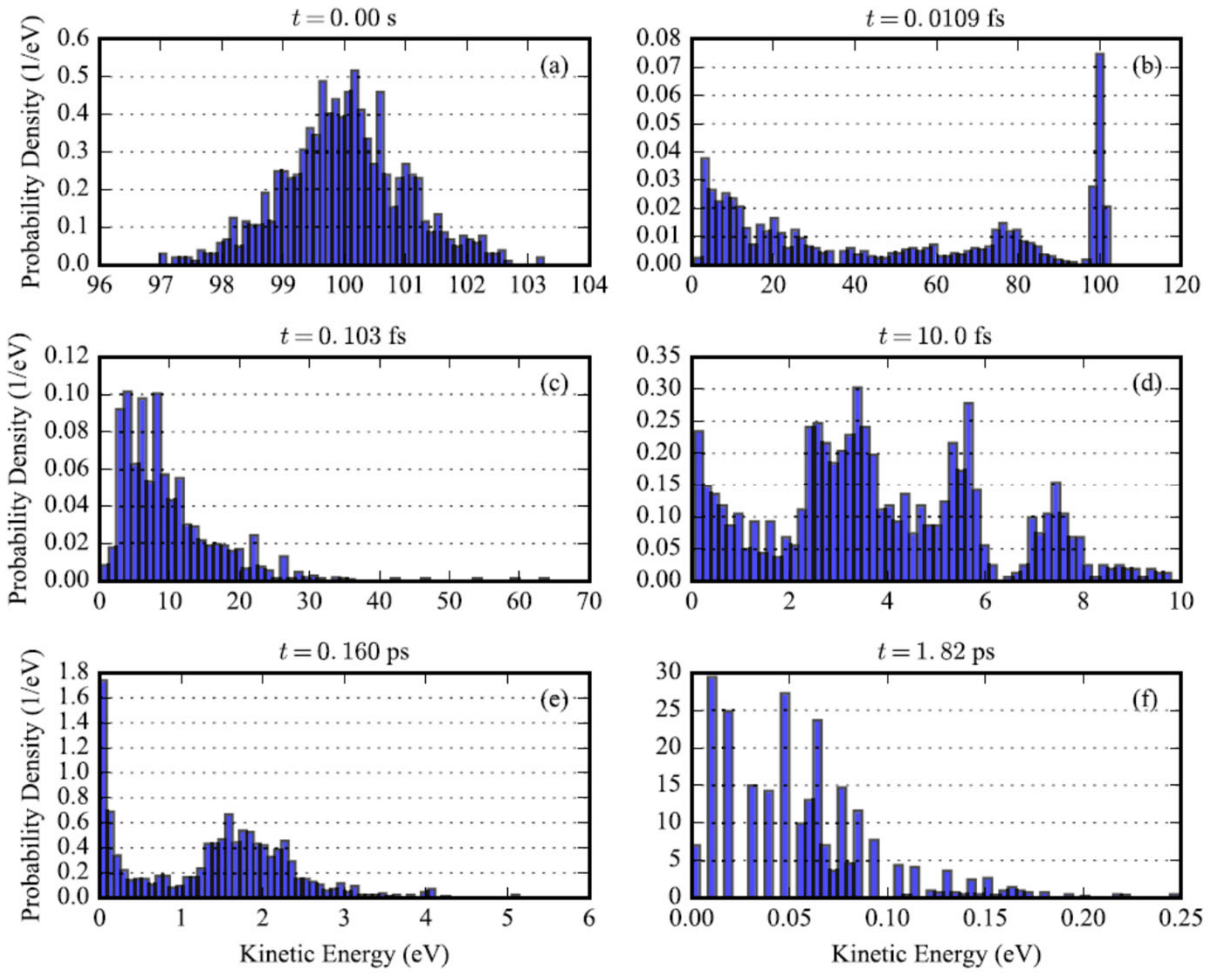


FIG. 3. The ratio of the uncertainty in the quasi-particle energy to its excitation energy as a function of p/p_0.

[1] J. J. Quinn, Phys. Rev. **126**, 1453 (1962).
[2] F. Capasso *et al*., J. Appl. Phys. **53**, 3324–3326 (1982).
[3] Y.-C. Chang *et al*., Appl. Phys. Lett. 42, 76–78 (1983).

Time evolution of the electron-energy distribution function in GaN

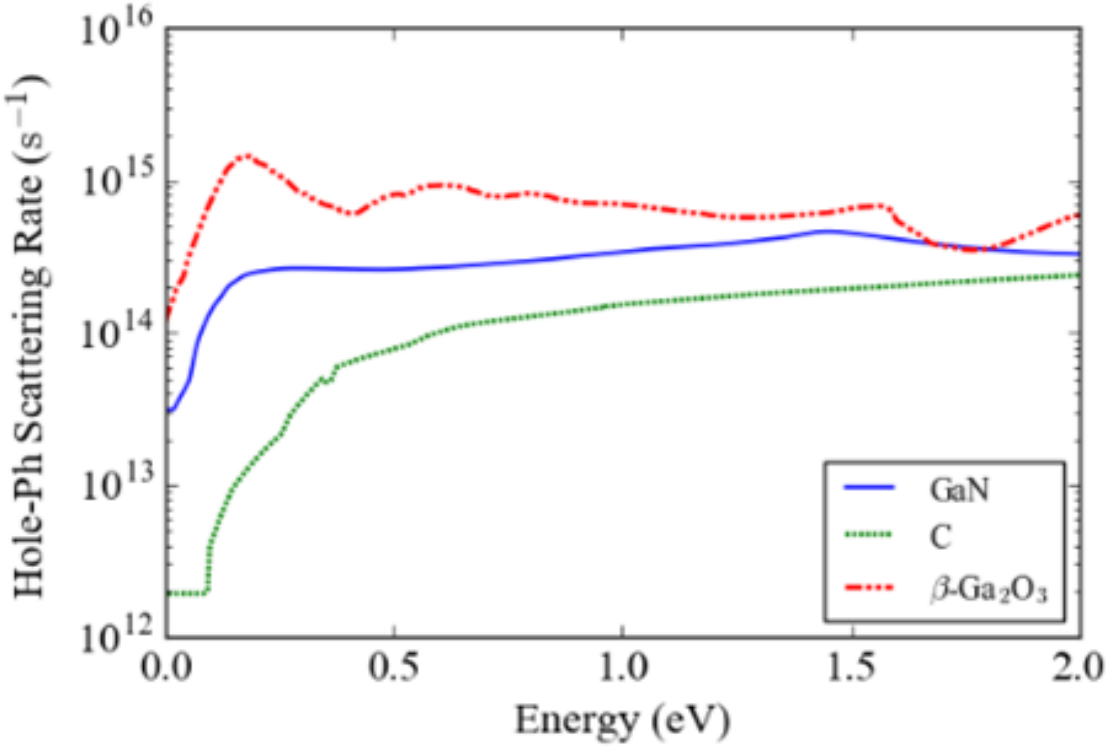


D. O. Nielsen *et al.*,
Phys. Rev. B **108**, 155203 (2023).

Hole-phonon scattering rates: Slow hole thermalization in C (diamond)

- Hole mobility (300K):
  - C (diamond, exp): 3,500 $cm^2/(Vs)$ [1]
  - GaN (wurtzite, theory): 52 $cm^2/(Vs)$ [2](?)
    (nearly intrinsic, exp): 170 $cm^2/(Vs)$ [3]
  - β-Ga_2O_3 (N doped, exp): ~ 23 $cm^2/(Vs)$ [4]

  Small hole mass in diamond, flat VBs in GaN and Ga_2O_3



[1] J. Isberg *et al.*, Science **297**, 1670 (2002).
[2] S. Poncé, D. Jena, and F. Giustino, Phys. Rev. B **100**, 085204 (2019).
[3] M. Rubin *et al.*, Appl. Phys. Lett. **64**, 64 (1994).
[4] C. Ma *et al.*, J. Mater. Chem. C **10**, 6673 (2022).