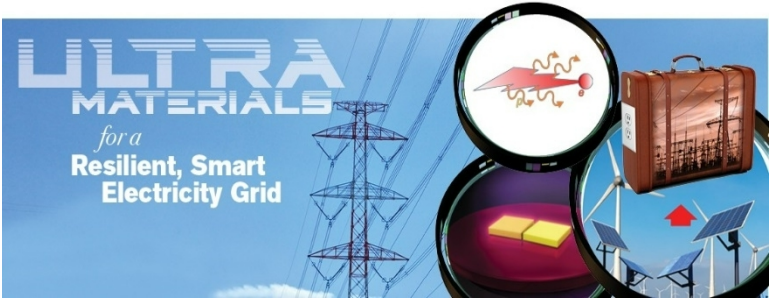


SAND2022-11378C

Ultrawide Bandgap Semiconductors: Influence of Material Properties on Power Device Performance

Stephen Goodnick, Jonah Shoemaker, Robert Nemanich
Arizona State University, Tempe, AZ, USA

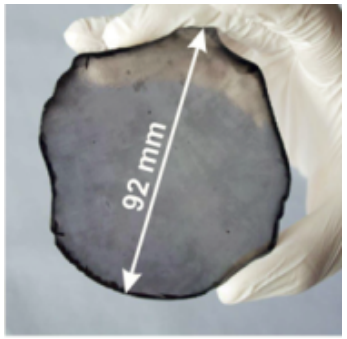
Robert Kaplar, Jack D. Flicker and Andrew Binder
Sandia National Labs, Albuquerque NM, USA

August 24, 2022

This work was supported as part of ULTRA, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

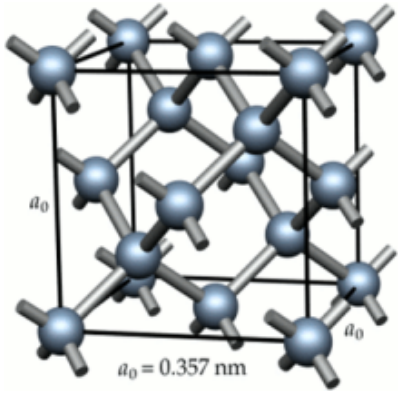
U.S. DEPARTMENT OF ENERGY | Office of Science

ULTRA Semiconductors



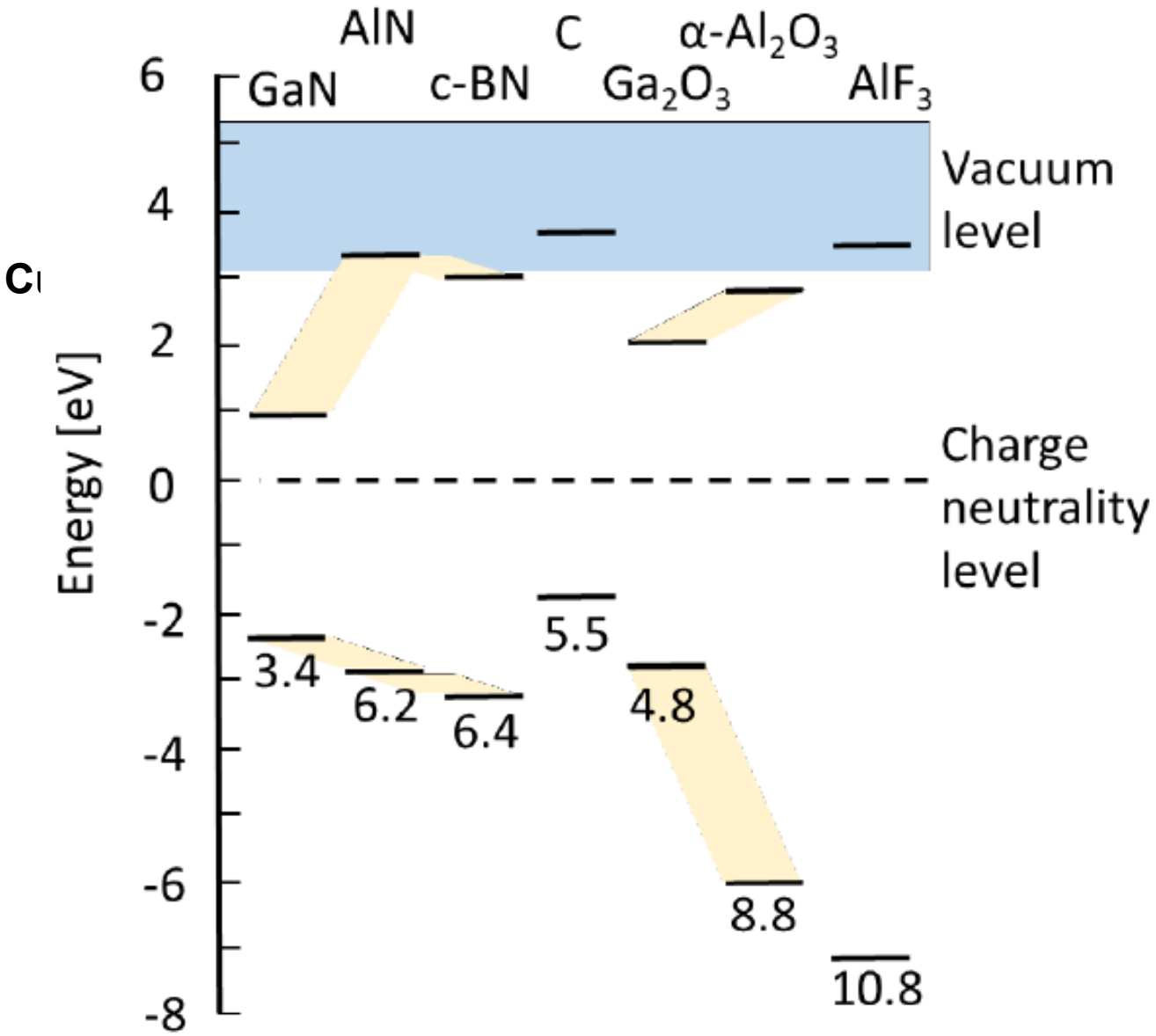
Augsburg Univ.

Diamond Cubic



- Eg = 5.5 eV
- sp^3 bonded carbon
- C – 6e
- Diamond Cubic

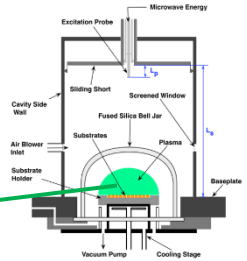
  a = 3.57 Å

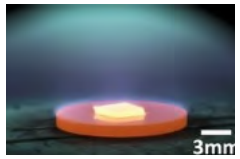


exaTech

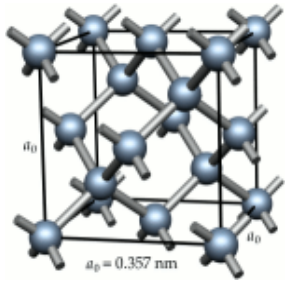
G. L. Doll, J. A. Sell, C. A. Taylor II, and R. Clarke, Phys. Rev. B, **43**, 6816 (1991).

ULTRA Semiconductor Synthesis

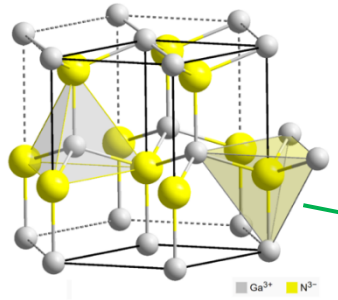




MPCVD

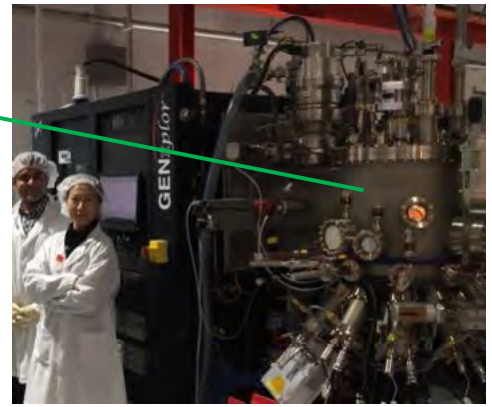


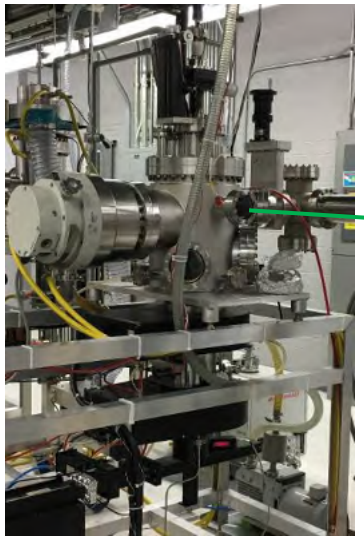
Diamond

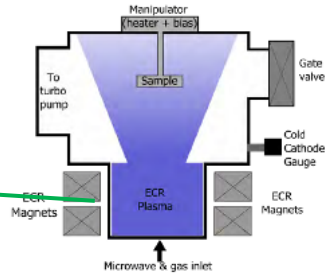


AlN and ($B_xAl_{1-x}N$)

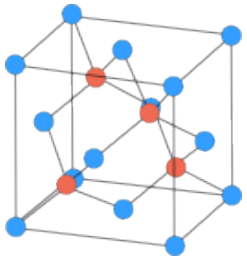
MBE



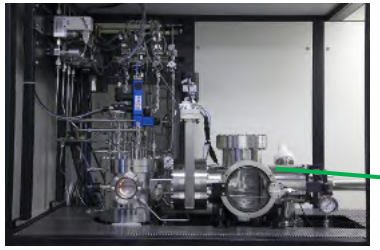




ECR-MPCVD



c-BN



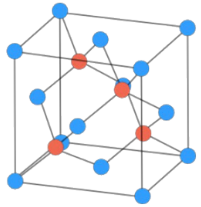
AlGaN

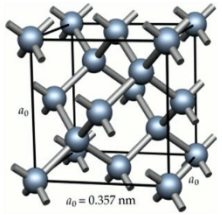
MOCVD

ULTRA EFRC

Mission: To achieve extreme electrical properties and phenomena through fundamental understanding of ultra wide bandgap materials, which will enable a resilient, smart electricity grid.


Wurtzite AlN


Cubic boron nitride (c-BN)



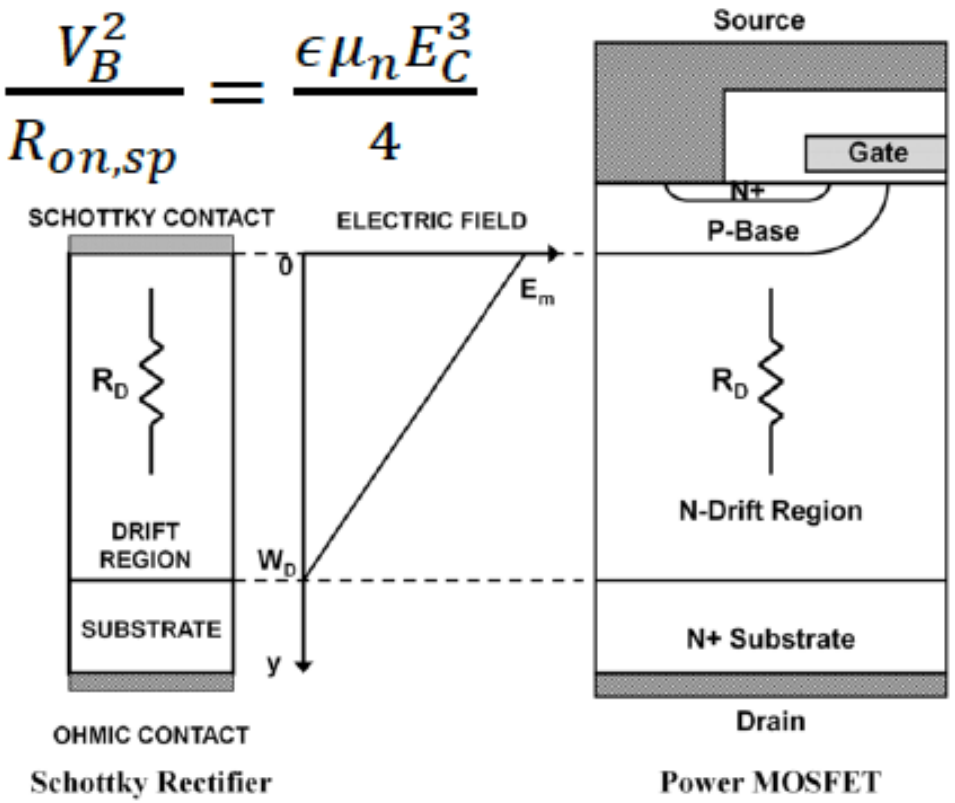
Diamond Cubic

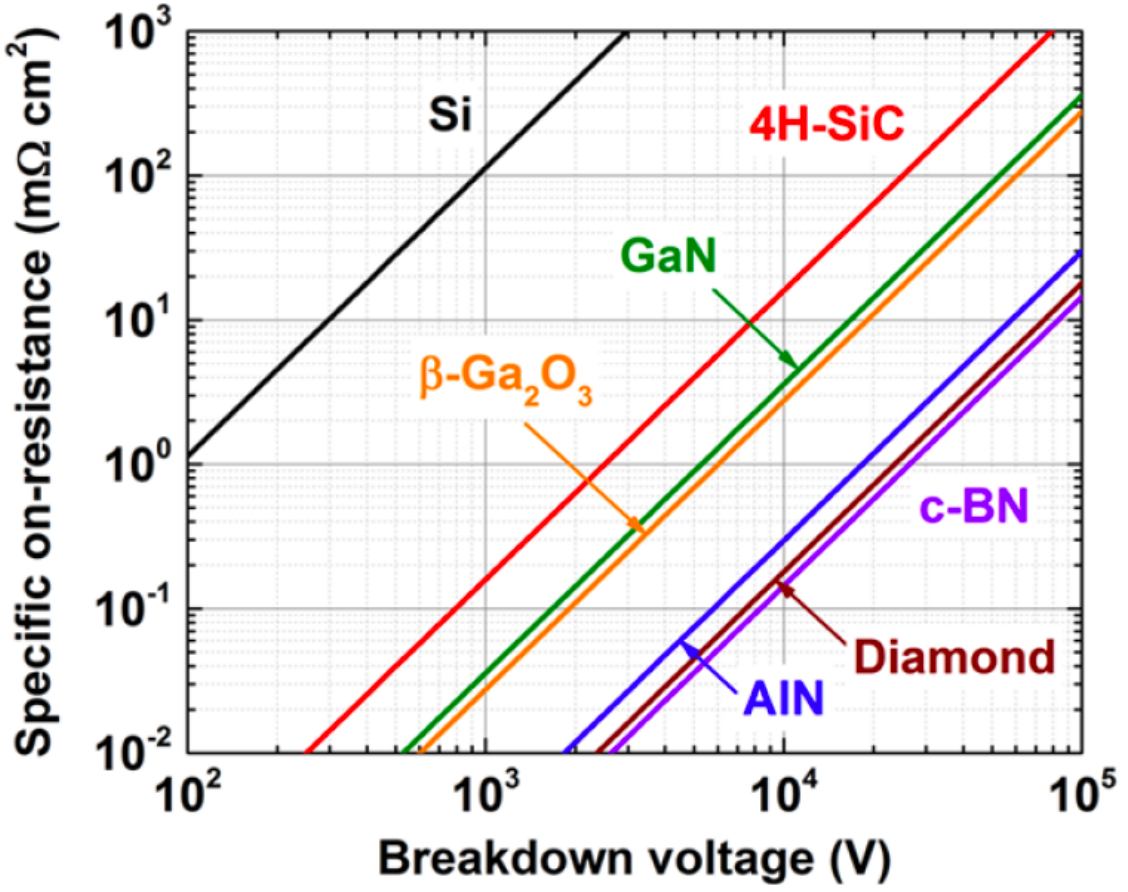
- **Methodology**
  - ➢ Close integration of theory and computational methods throughout
  - ➢ Materials synthesis, defect and impurity physics
  - ➢ Interfaces, atomic scale and electronic states characterization
  - ➢ High field electronic transport and breakdown characterization
  - ➢ Thermal transport theory and measurement
- **Future Grid Co-Design Ecosystem**
  - ➢ Provides a knowledge base enabling communication across all levels of the technology

Impact on Power Electronics: Baliga* Figure of Merit

There are two main parameters of importance for power electronics, the breakdown voltage (related to the critical field, E_C for impact ionization), and the specific on-resistance

$$\frac{V_B^2}{R_{on,sp}} = \frac{\epsilon \mu_n E_C^3}{4}$$





*Baliga B J 1982 Semiconductors for high voltage vertical channel field effect transistors J. Appl. Phys. 53 1759–64

Impact on Power Electronics: Baliga* Figure of Merit

The *unipolar* FOM is widely used to compare materials of power electronic applications, based on two important quantities: the reverse breakdown voltage, V_B, and the forward specific on-resistance, $R_{on,sp}$:

$$FOM = \frac{V_B^2}{R_{on,sp}}$$

For Ohmic conduction, $R_{on,sp}$ is connected to the semiconductor material through the electron (hole) density, $n(p)$, the carrier mobility, $\mu_{n,p}$, and the drift region width, W_d:

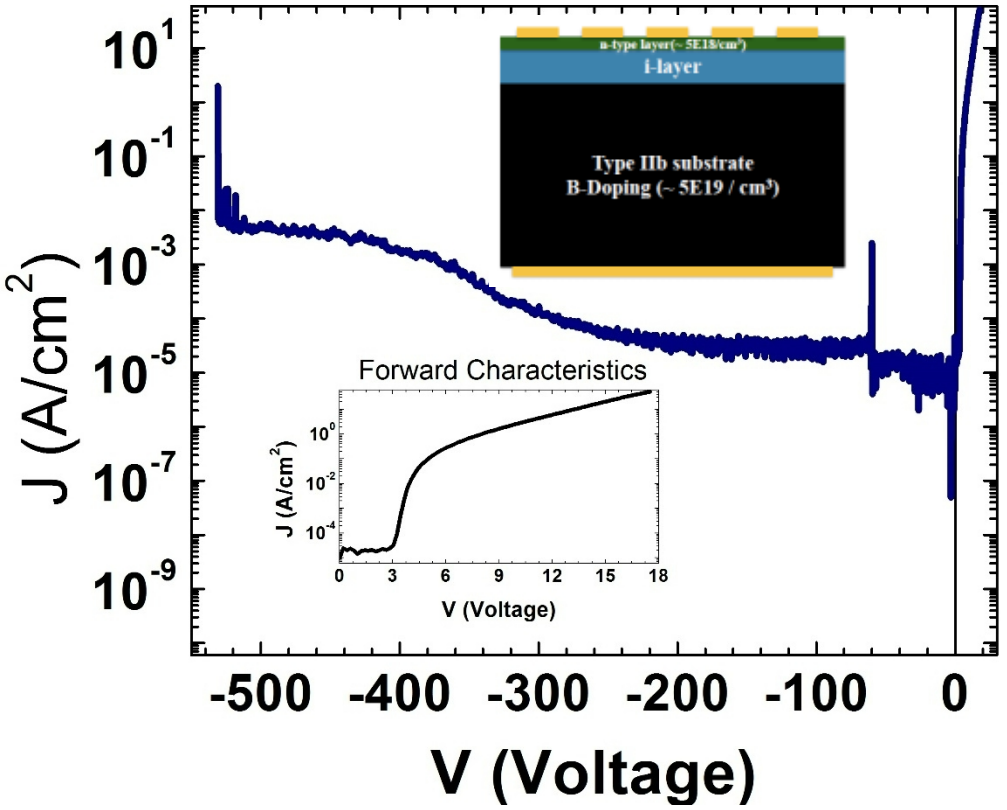
$$R_{on,sp} = \frac{W_d}{q\mu_{n,p}(n,p)}$$

The breakdown voltage depends on the breakdown (critical) field, $V_B = \eta \mathcal{E}_{cr} W_d$, which varies as the square of the bandgap

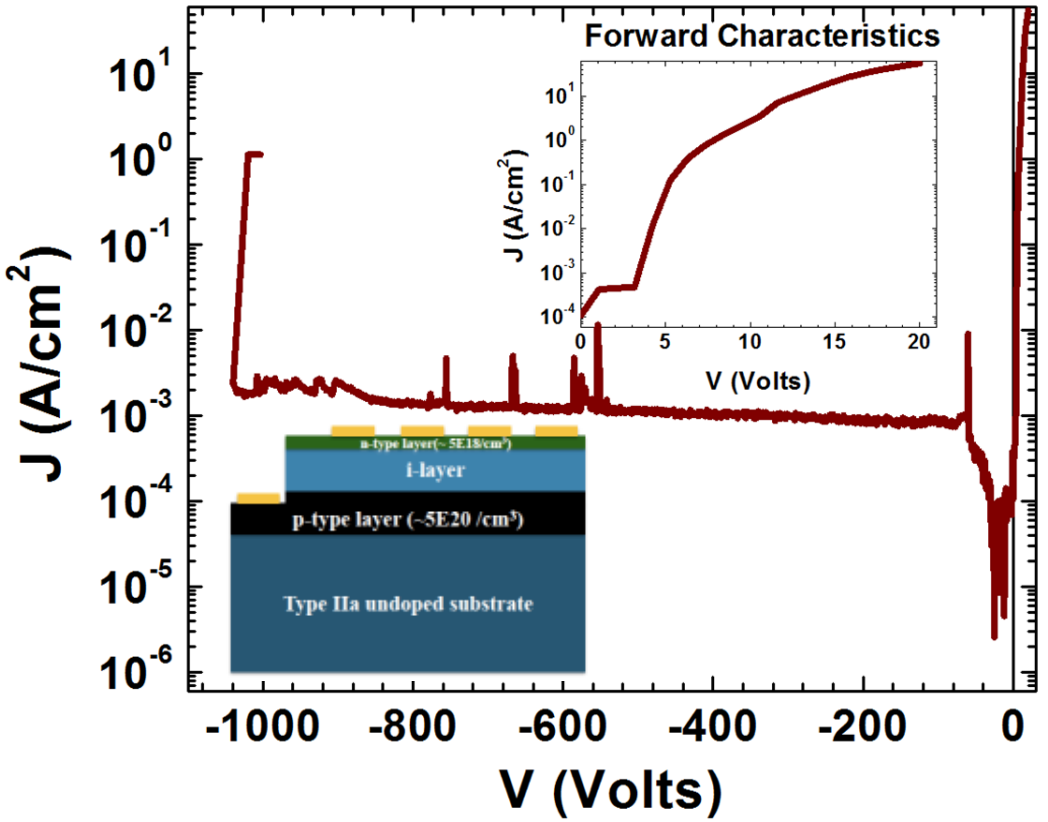
	Narrow		Wide	ULTRAs – New class of materials			
	Si	4H-SiC	GaN	ß-Ga_2O_3	Diamond	h-AlN	h-BN
Bandgap (eV)	1.12	3.26	3.4	4.9	5.5	6.2	6.4
Breakdown Field (MV/cm)	0.3	2.5	3.8	8	10	16	12
Baliga's figure of merit (FOM)	**1**	**183**	**535**	**3444**	**9000**	**9797**	**1678**
	Traditional		**New**	**Emerging Technology**			

From M. Kuball, EFRC highlight 2020

Breakdown in Diamond SPIN Diodes



- Type IIb substrate with ~ 3.5 micron i-layer
- Forward Current Density ~ 50 A/cm^2 at 17 V
- Breakdown voltage ~ 530 V at 1E-2 A/cm^2



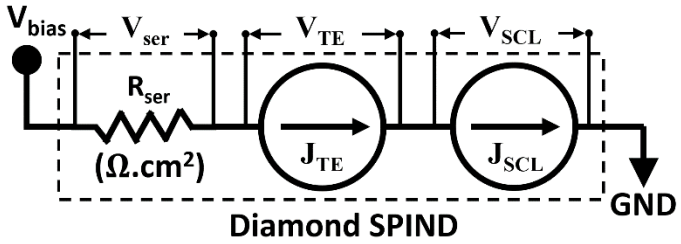
- Type IIa substrate with ~ 8.5 micron i-layer
- Forward Current Density ~ 55 A/cm^2 at 20 V
- Breakdown voltage ~ 1040 V at 1E-3 A/cm^2

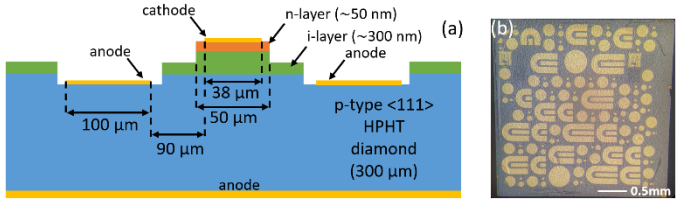
< 10 /

M. Dutta, F. Koeck, R. Hathwar, S. Goodnick, R. Nemanich, and S. Chowdhury, "Demonstration of diamond-based Schottky p-i-n diode with blocking voltage > 500 V," IEEE Elect Device Lett., 37, 1170 (2016)

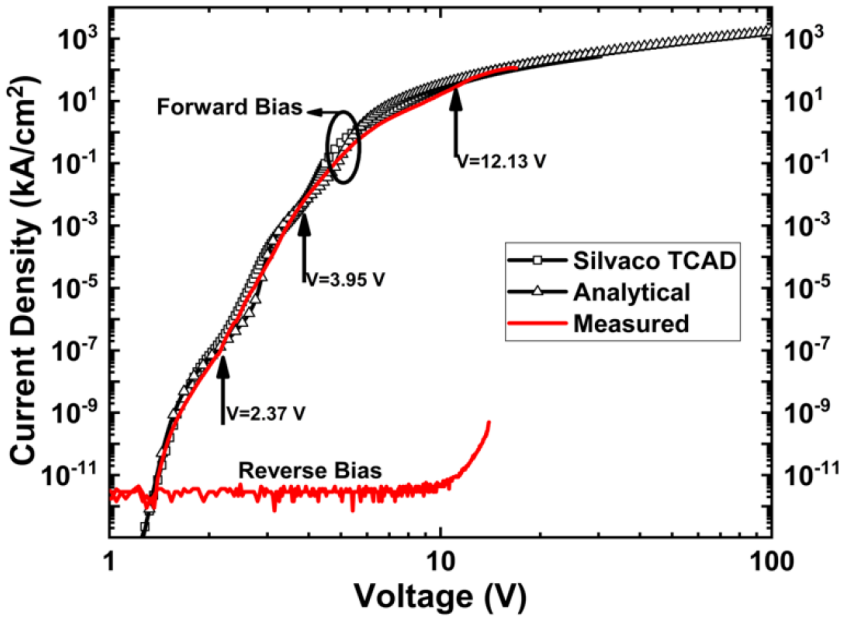
Forward Characteristics of Diamond SPIN Diodes

Record forward current (116 kA/cm^2) measured in Schottky PIN diodes. Strong evidence of Mott-Gurney space charge limited current regime in forward bias including trap effects.

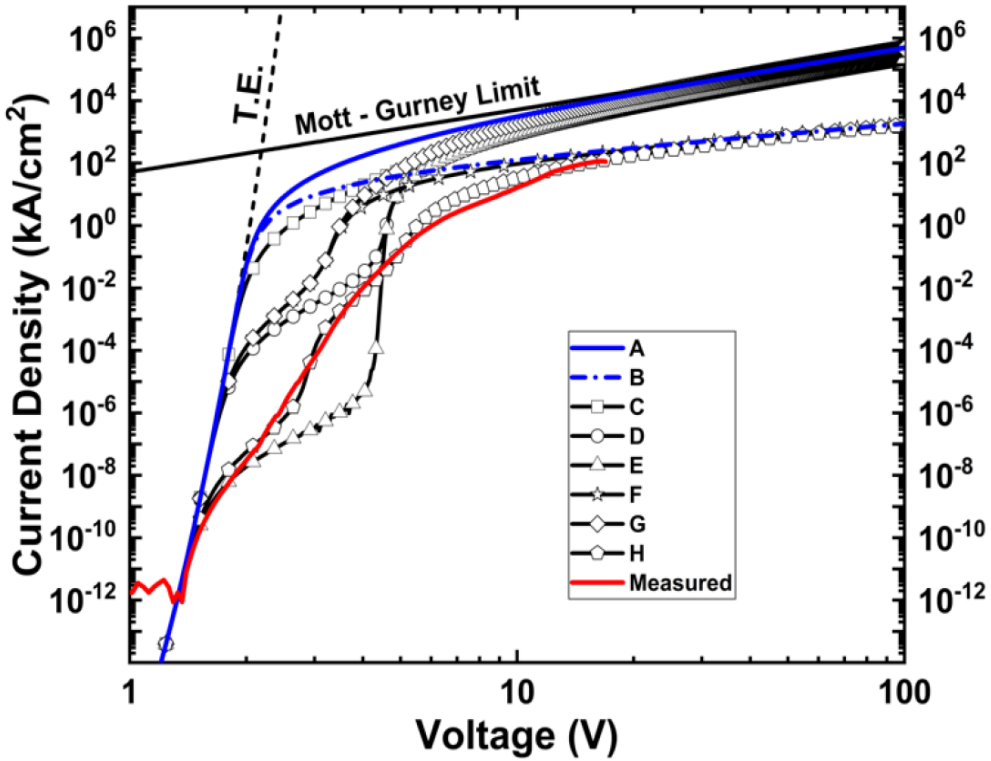




$$J = \frac{9}{8}\epsilon\mu_p\frac{V^2}{d^3}$$



3 Trap model explains jumps in the J-V characteristics, and limitations compared to ideal behavior

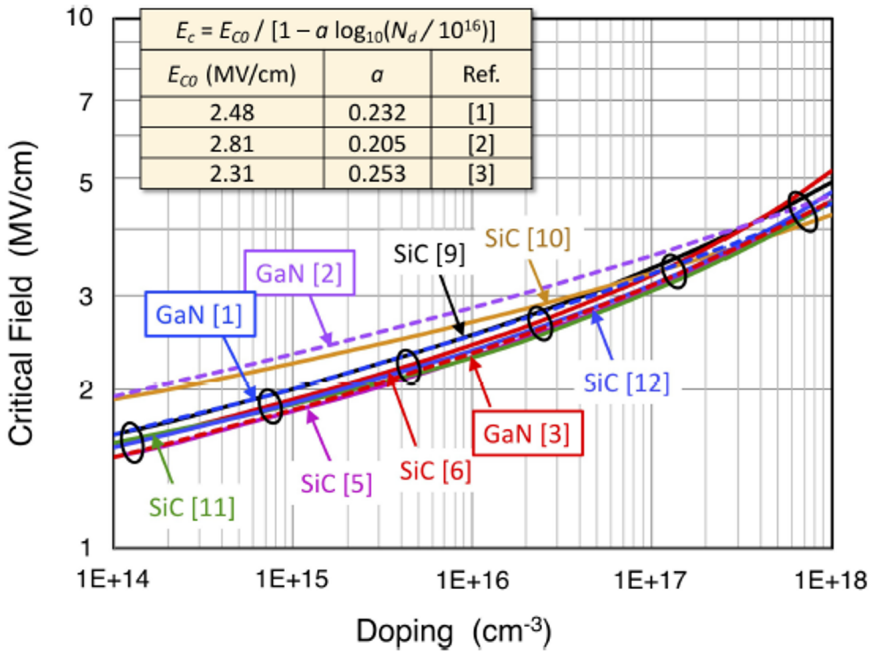


H. Surdi, F. A. M. Koeck, M. F. Ahmad, T. J. Thornton, R. J. Nemanich, and S. M. Goodnick, *IEEE Trans. Elec. Dev.* 69(1), 254-261 (2022)

Shortcomings of Simple FOM Equation

- **There is no such thing as a single "Critical Field" for a semiconductor material**
  - Breakdown field depends on doping and temperature
  - Also depends on drift region geometry, i.e. punch-through vs non-punch-through
- **Treatment is inherently one-dimensional**
  - Vertical drift region only (lateral FOM can be derived)
  - Impact ionization is anisotropic
  - Misrepresents real devices where 2- and 3-D effects typically dominate (e.g. edge terminations)
- **Transport is over-simplified**
  - Assumes complete dopant ionization, which is universally untrue for UWBGs
  - Assumes simple low-field drift transport only

J. A Cooper and D. T. Morisette,
EDL 41(6), 892 (2020)



[1] L. Cao et al., Appl. Phys. Lett. 112, 262103 (2018)
[2] D. Ji et al., Appl. Phys. Lett. 115, 073503 (2019)
[3] T. Maeda et al., J. Appl. Phys. 129, 185702 (2021)

Optimal Drift Region Design

- **For a given drift region thickness W_d:**
  - Select a doping level $N_{D,A}$
  - Evaluate the ionization integral to determine the breakdown voltage for that (W_d, $N_{D,A}$ pair):

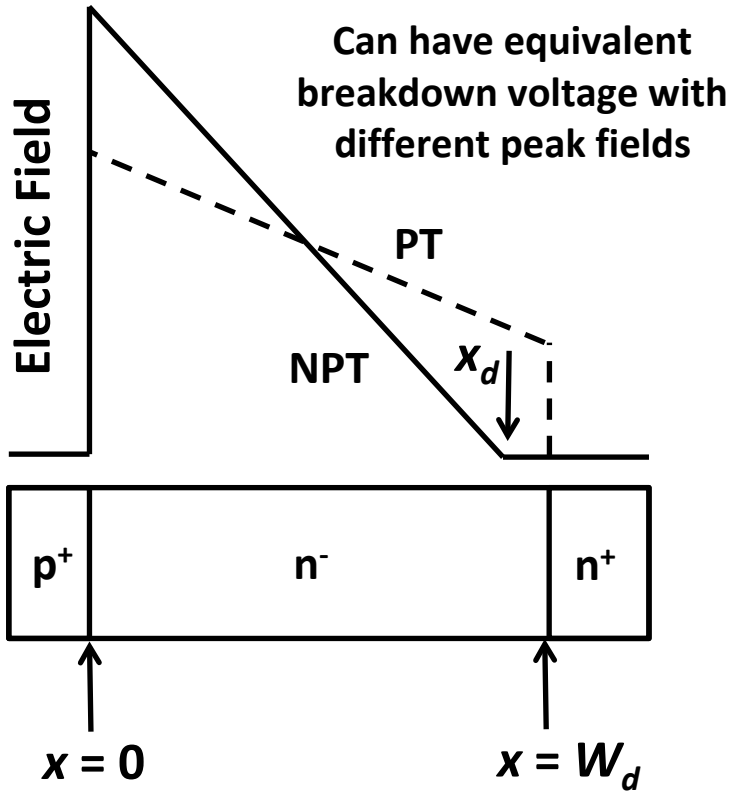
$$\int_0^{x_d} \alpha(E(x)) \exp\left[\int_x^{x_d} \left(\beta(E(x')) - \alpha(E(x'))\right) dx'\right] dx \rightarrow 1$$

  - Determine the specific on-resistance for that (W_d, $N_{D,A}$ pair):

$$R_{on,sp} = \frac{W_d}{q\mu_{n,p} n(or\ p)}$$

Does not necessarily equal N_D or N_A, to be discussed later

  - Iterate the doping $N_{D,A}$ to generate a curve of ($R_{on,sp}$, V_B) points for that W_d



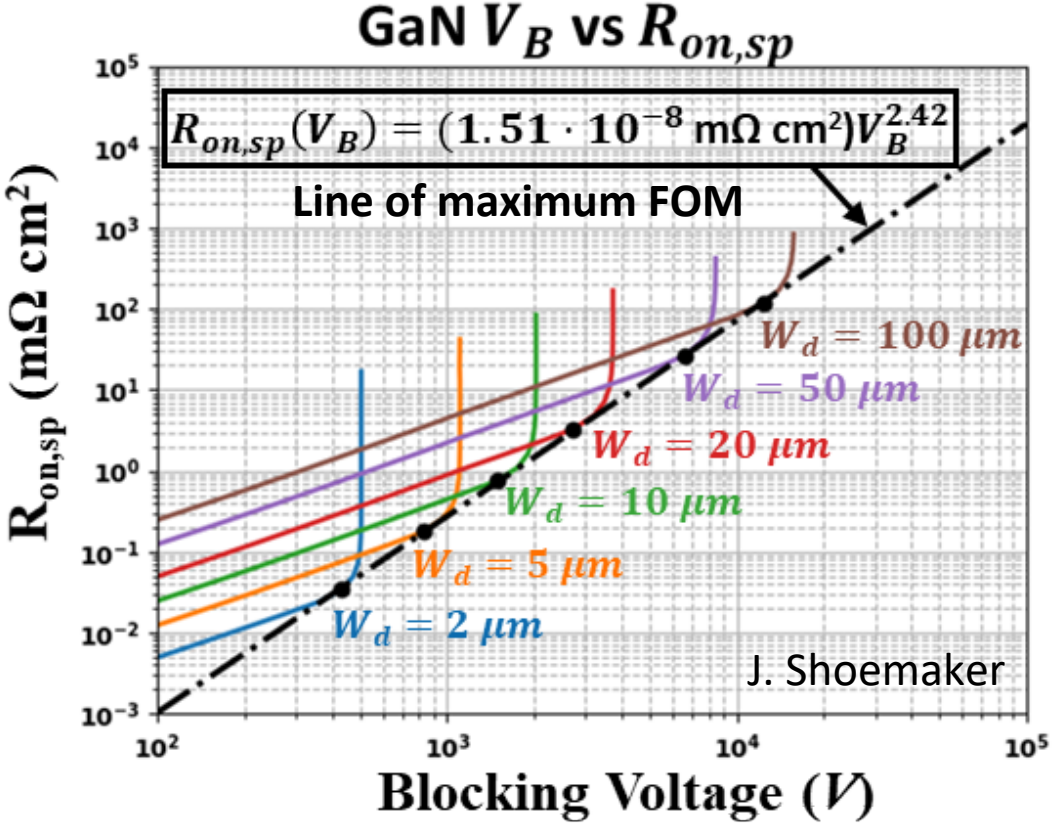
Based on method in J. A Cooper and D. T. Morisette, EDL 41(6), 892 (2020)

Optimal Drift Region Design

- **Iterate the drift region thickness W_d**
  - Repeat the procedure from the previous slide for each W_d to generate additional curves of $R_{on,sp}$ vs V_B
  - For each such curve, determine the optimal point based on maximizing the unipolar FOM:

$$FOM = \frac{V_B^2}{R_{on,sp}}$$

  - Draw a line through each of these optimal points to generate a curve of constant FOM – this is the limit for the material being evaluated



Based on method in J. A Cooper and D. T. Morisette, EDL 41(6), 892 (2020)

Impact Ionization Coefficients

Impact ionization rate from screened Coulomb interaction:

$$\frac{1}{\tau} = \frac{2\pi}{\hbar}\frac{V^3}{(2\pi)^9}\sum_{n_1,n_2n_2,}\iiint dk_1,dk_2dk_2,$$

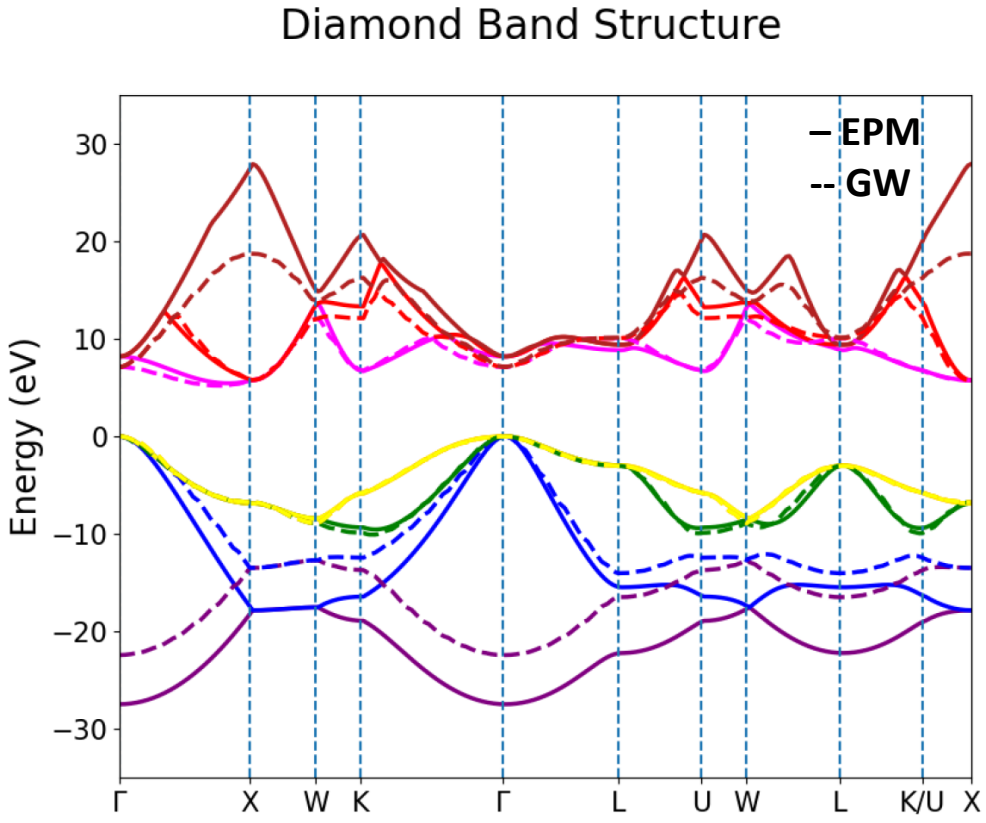
Integration across the hot carrier final state k_1, and cool carrier initial and final states k_2 and k_2,

$$\times |M(n_1',k_1',n_2',k_2';n_1,k_1,n_2,k_2)|^2$$
$$\times \delta\big(E(k_1,)+E(k_2,)-E(k_1)-E(k_2)\big)$$

$$|M|^2 = |M_D|^2 + |M_E|^2 - (M_D^* M_E + M_D M_E^*)/2$$

Sum across all four states' reciprocal lattice vectors requires full knowledge of the band structure and wave-functions

$$M_D = \sum_{G_1,G_2,G_1',G_2,} a^*_{n_1',k_1,}(G_1')a^*_{n_2',k_2,}(G_2')$$
$$\times a_{n_1,k_1}(G_1)\,a_{n_2,k_2}(G_2)\frac{e^2}{4\pi\epsilon(q_D,\omega_D)q_D^2}$$
$$\times \delta(k_1,+G_1,+k_2,+G_2,-k_1-G_1-k_2-G_2)$$



J. Shoemaker

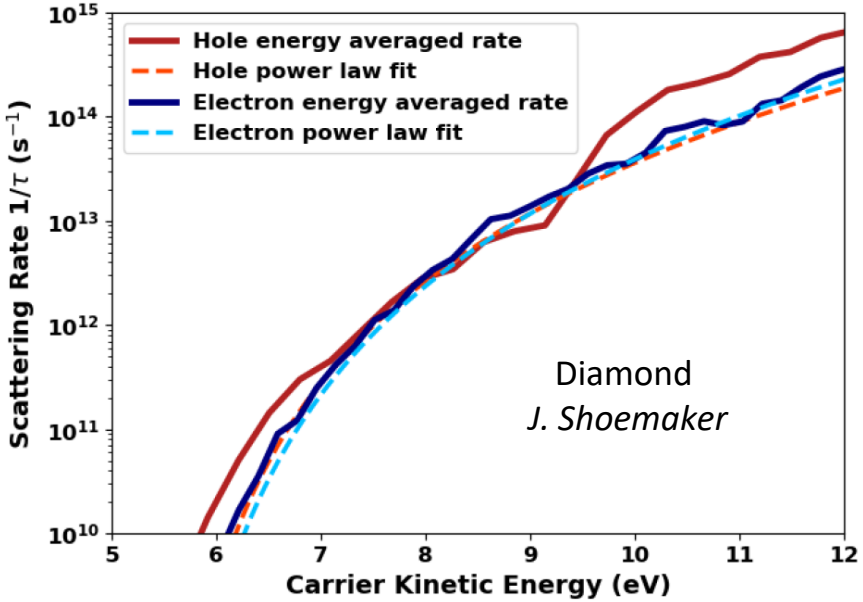
Impact Ionization Coefficients

- Use first principles calculations to determine electronic bandstructure
- Full band impact ionization rates are calculated from Fermi's Golden Rule
- Used to calculate the impact ionization coefficients using full band Monte Carlo simulation

$$\alpha_i(\epsilon) = \frac{1}{N\bar{v}_i(\epsilon)} \frac{dn_i(\epsilon)}{dt}$$

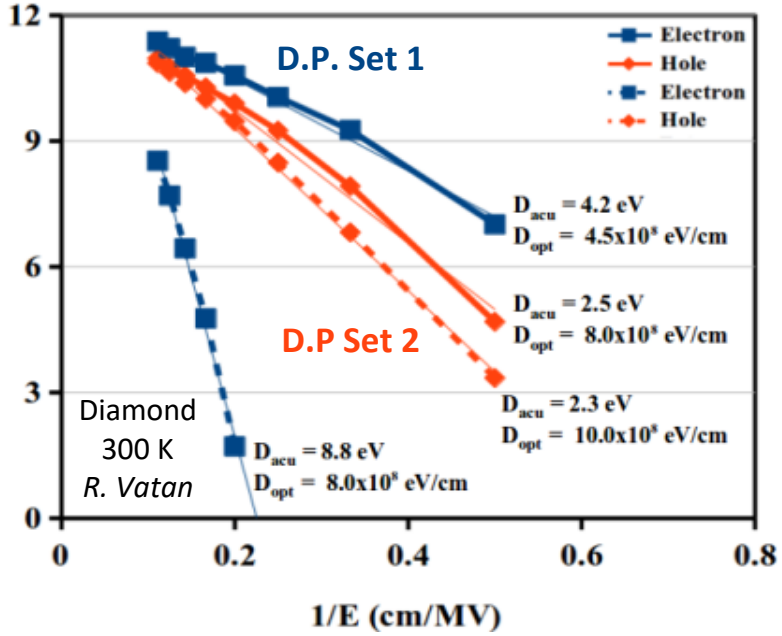
Scattering rate power law fits:

$$1/\tau_h(\varepsilon) = 3.67 \cdot 10^{10}(\varepsilon - \varepsilon_{th})^{4.54}$$
$$1/\tau_e(\varepsilon) = 2.44 \cdot 10^{10}(\varepsilon - \varepsilon_{th})^{4.86}$$



Chynoweth equation:

$$\alpha(E) = \alpha_o exp\left(-\frac{E_0}{E}\right)$$



- **Values for other materials from literature also used* – calculations ongoing**
- **Comparison between theory and experiment is lacking for UWBGs (and even GaN)**

* E. Bellotti and F. Bertazzi, J. Appl. Phys. 111, 103711 (2012)

Low-Field Transport and Mobility

The mobility of non-alloy materials is computed according to the Caughy-Thomas fit:

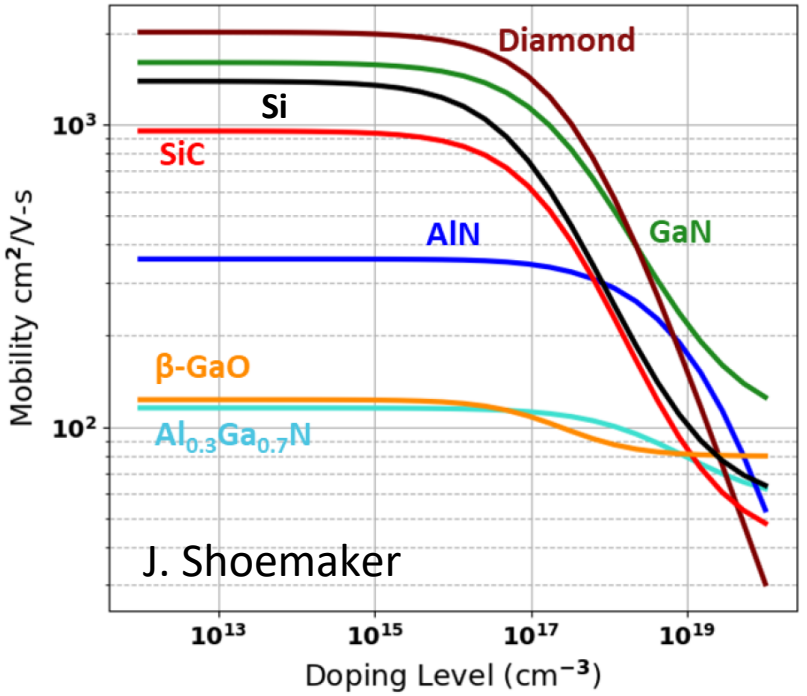
$$\mu(N_{D,A}) = \mu_{min} + \frac{\mu_{max} - \mu_{min}}{1 + \left(\frac{N_{D,A}}{N_{ref}}\right)^{\alpha}}$$

The parameters μ_{min}, μ_{max}, N_{ref}, and α are provided by empirical fits to experimental data and have been obtained from literature for all the materials used.

For $Al_xGa_{1-x}N$, the alloy mobility is computed and added to a linear interpolation of the GaN and AlN mobilities using Mathieson's Rule:

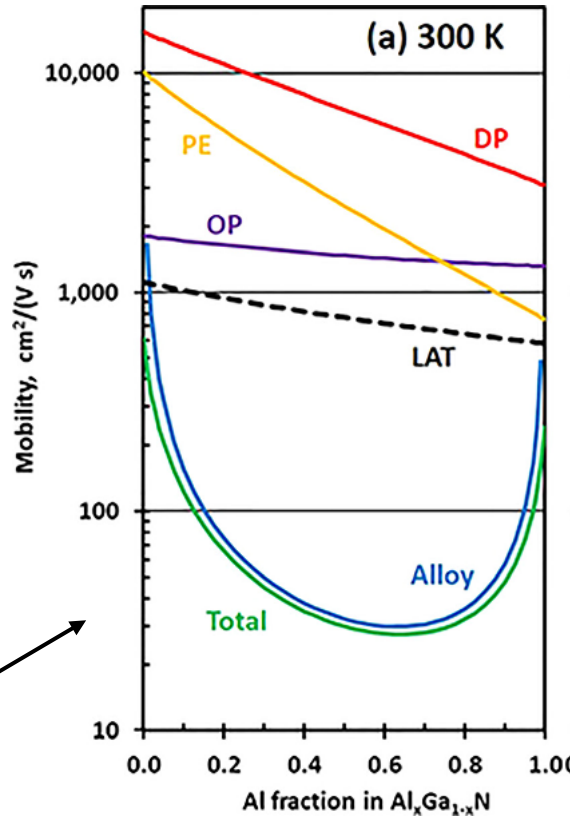
$$\mu_{alloy}(x) = \frac{32q\hbar^4}{9\sqrt{2}\pi^{\frac{3}{2}}\Omega x(1-x)(\Delta E)^2(m^*)^{\frac{5}{2}}(kT)^{\frac{1}{2}}}$$

Mobility from Caughy-Thomas Model



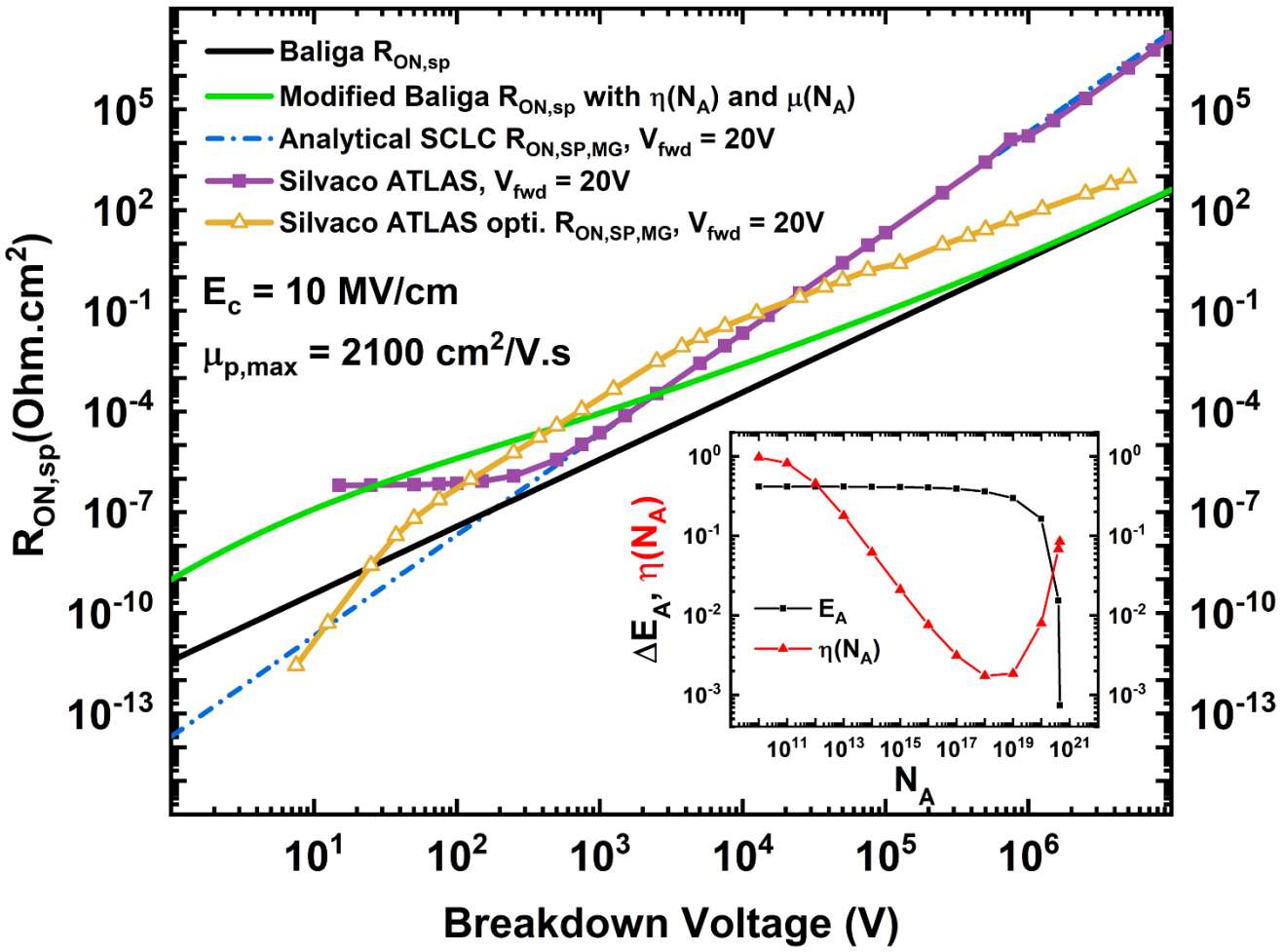
$$\frac{1}{\mu_{Al_xGa_{1-x}N}} = \frac{1}{\mu(N_{D,A})} + \frac{1}{\mu_{alloy}(x)}$$

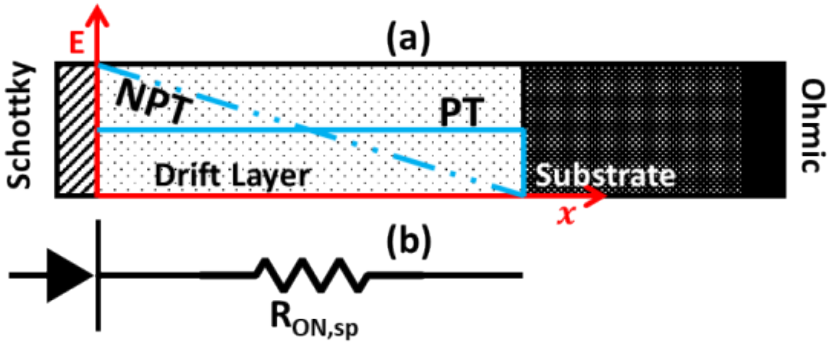
Calculated AlGaN mobility



M. E. Coltrin and R. J. Kaplar, J. Appl. Phys. 121, 055706 (2017)

Power Electronic Figure of Merit (FOM) Revisited





Incomplete Ionization

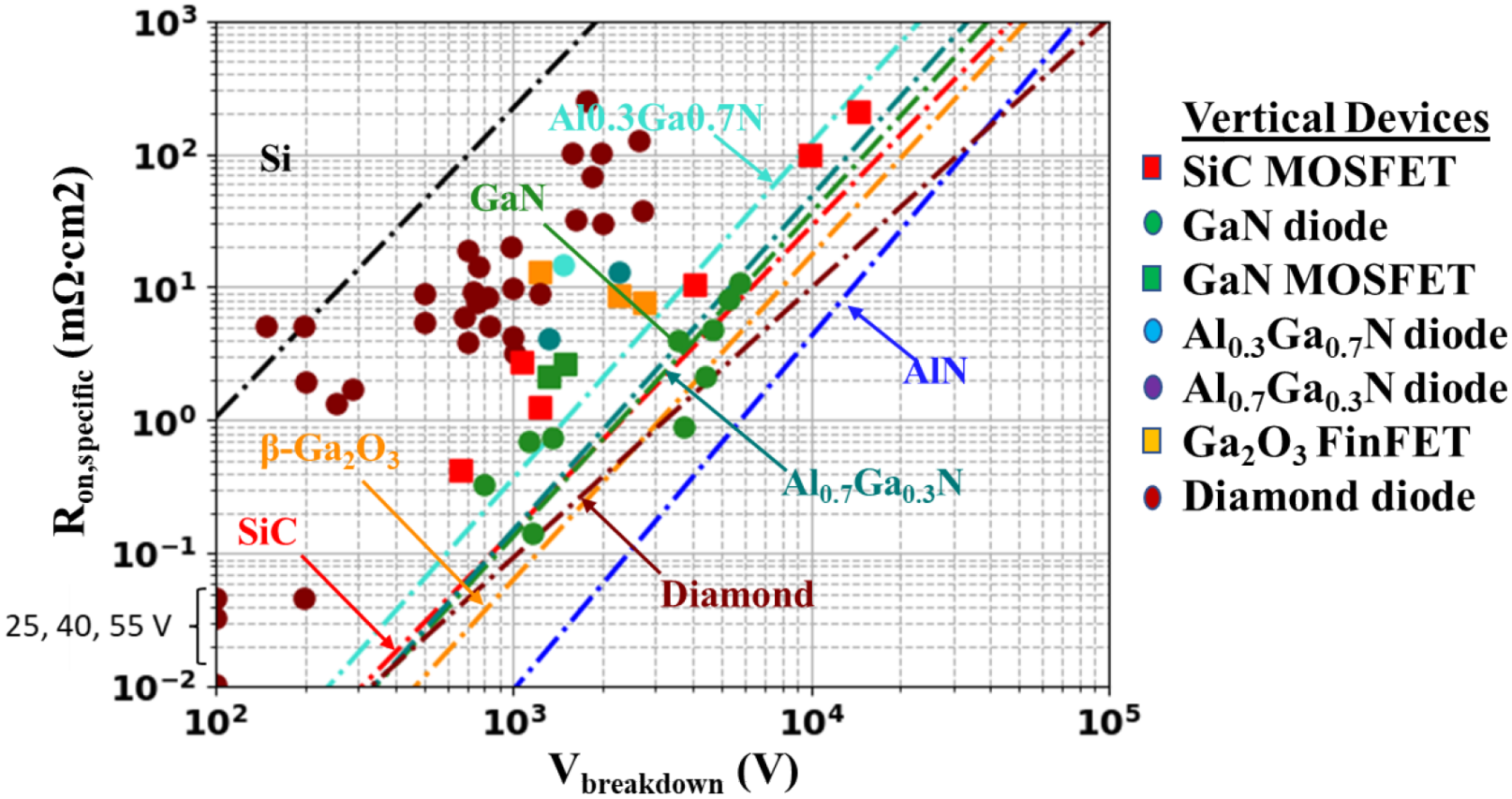
$$R_{ON,sp} = \frac{d}{q\mu(N_A^-)N_A^-}$$

Mott-Gurney

$$R_{ON,sp,MG} = \frac{4}{9\epsilon_r\epsilon_0\mu}\frac{d^3}{V}$$

Note: FOM no longer given by $\frac{V_B^2}{R_{on,sp}}$ for non-Ohmic I-V

Comparison Between Materials and to Experimental



Data points taken from A. J. Green, J. Speck, G. Xing, et al., "β-Gallium Oxide Power Electronics," APL Mater. 10, 029201 (2022), and various other references

Other FOMs Under Investigation

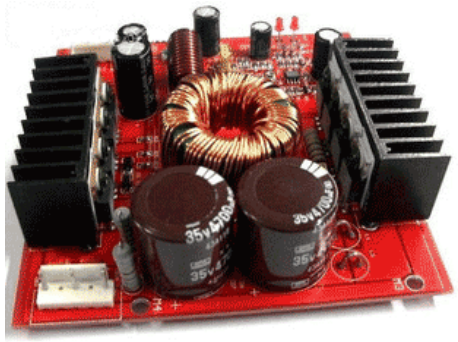
$$P_{loss,min} = \frac{4I_{rms}(V_B V_D)^{3/4}\sqrt{\frac{kI_D f}{i_{g,av}}}}{E_C\sqrt{\mu}}$$

Huang Material Figure of Merit

Presently being evaluated

$$\frac{f}{E_C^2\mu} = \text{Constant}$$

Power Density ~ f
~ $E_C^2\mu$ = HMFOM^2

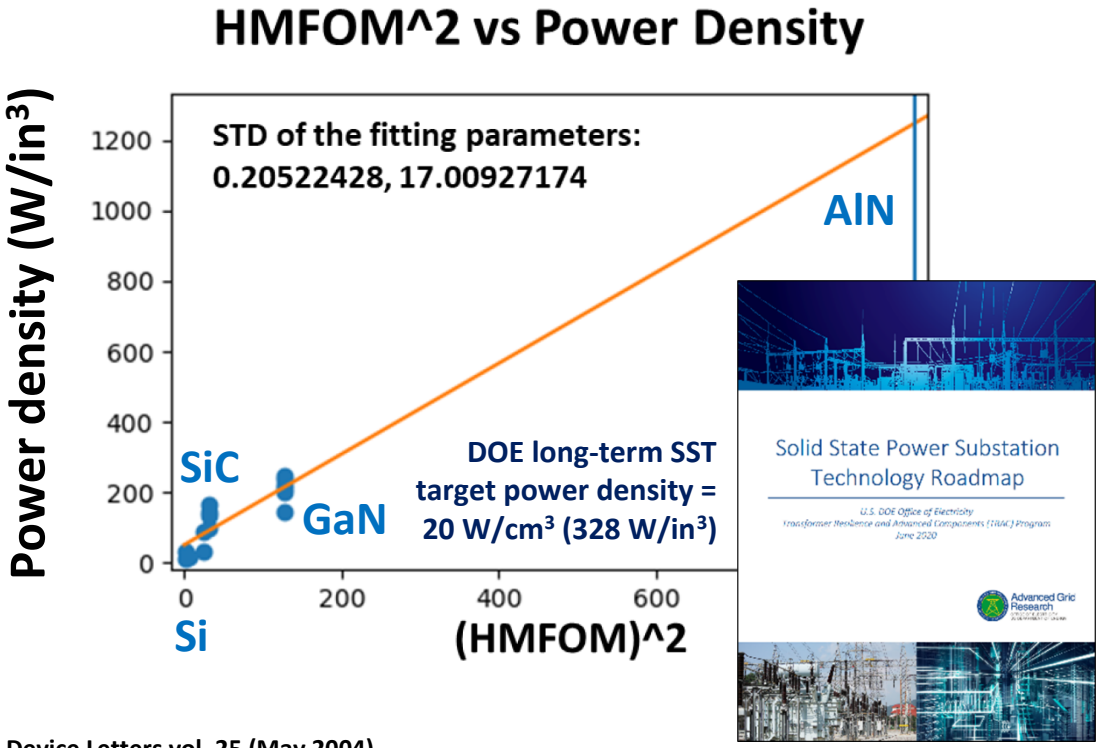


Si-based converter

WBG-based converter

UWBG-based converter

Need to also take into account thermal properties – other FOMs are applicable



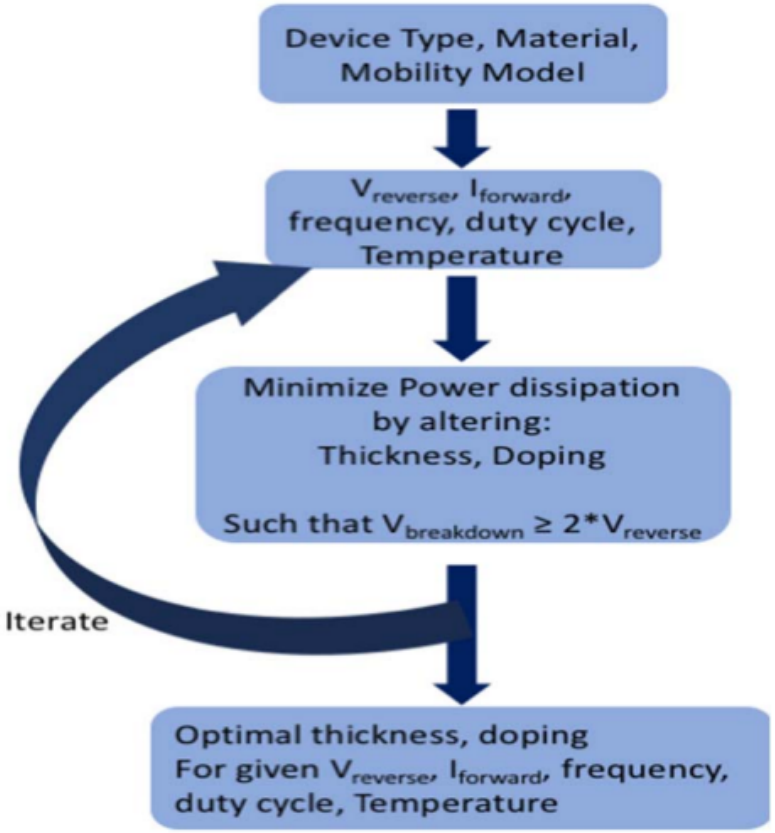
Based on analysis in R. J. Kaplar, J. C. Neely, et al., IEEE Power Electronics Magazine (March 2017) and A. Q. Huang, IEEE Electron Device Letters vol. 25 (May 2004)

PIN and SBD Diode Power Loss Optimization

- For a given set of operating parameters, the doping level and drift thickness are optimized to minimize power loss:

$$P_{total} = P_{forward} + P_{reverse} + P_{dynamic} + P_{displacement}$$

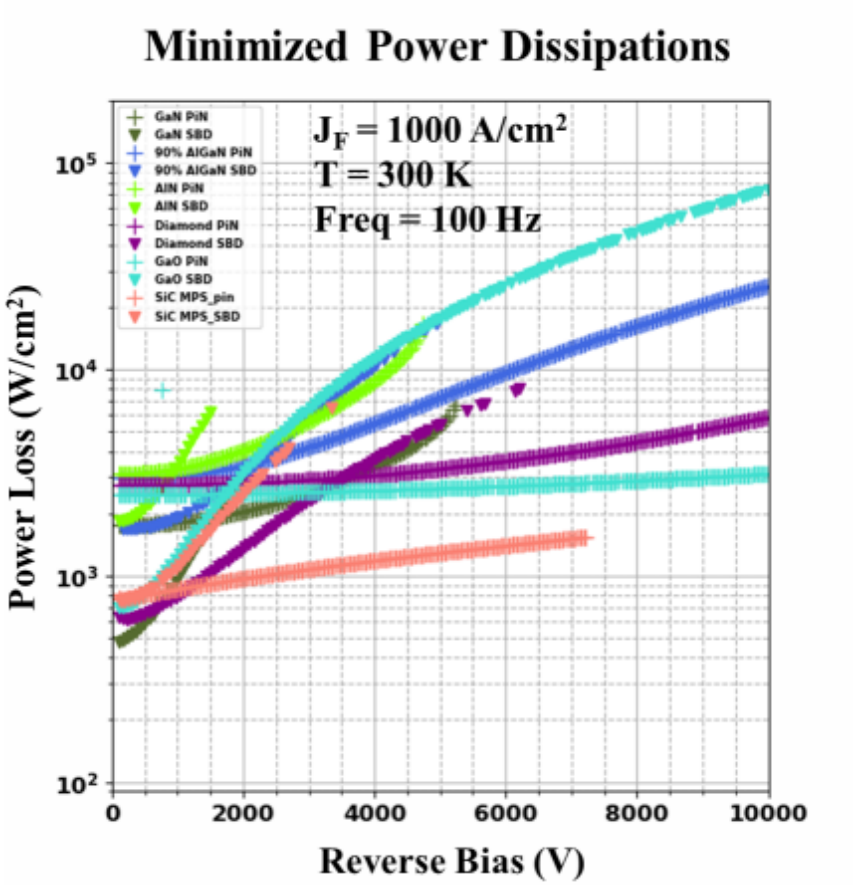
- The temperature- and doping-dependent mobilities are calculated theoretically or with empirical models fit to experiment
- The temperature-, doping-, and drift thickness-dependent critical fields are calculated from the ionization integral*
- UWBG-specific effects such as incomplete ionization and space-charge limited current are included

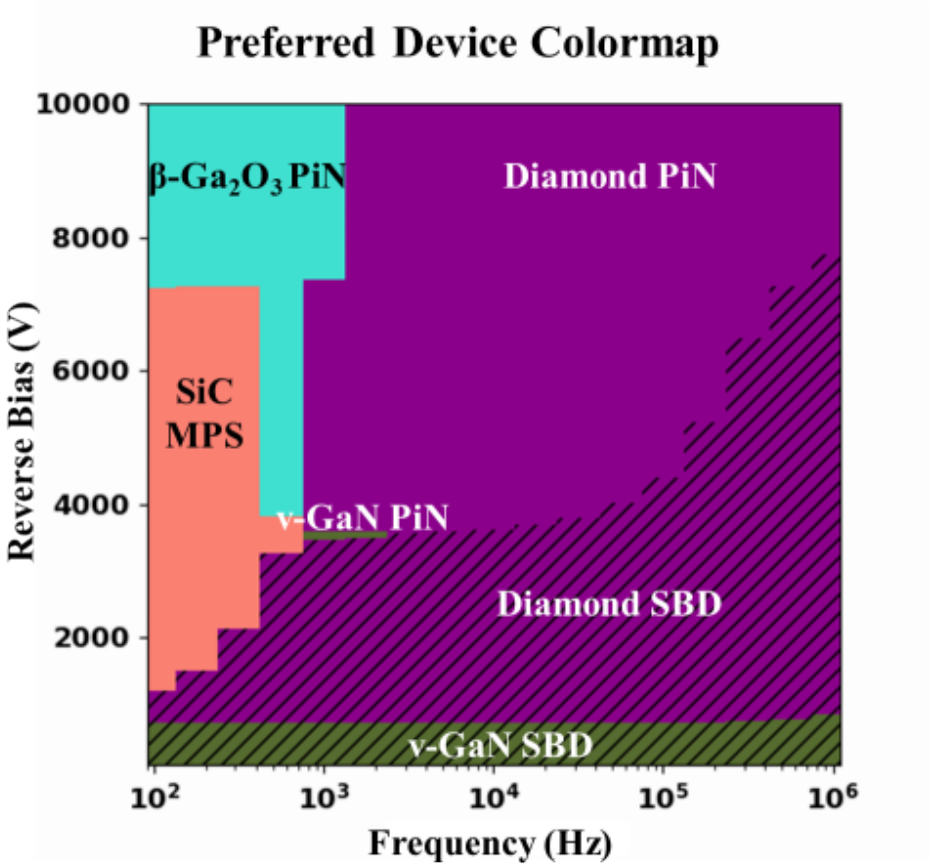


*J. Cooper et al., EDL 41(6) 892 (2020)

PIN and SBD Diode Power Loss Optimization

- The UWBG material and diode type (PIN or Schottky) that produces the lowest power loss for each reverse bias and frequency is plotted in a color-map





Summary

- **Ultra-materials ($E_g > 5\ eV$) hold promise for achieving high Figure of Merit (FOM) for power electronics applications**
- **The Baliga FOM relates semiconductor material properties to device performance**
  - Conventional approach to calculating FOM has been over-simplified, and this work attempts to correct some of the shortcomings of particular importance for UWBGs
  - Evaluate breakdown and optimal drift region design by evaluating ionization integral, utilizing the impact ionization coefficients for the material
  - Calculate impact ionization coefficients using full-band Monte-Carlo simulation
  - Incorporate doping-dependent mobility model, as well as non-ohmic transport
  - Evaluate incomplete dopant ionization
  - Other FOMs consider effects of frequency and power dissipation relevant to actual power electronic applications

Thanks!