TCAD Parameters for 4H-SiC: A Review

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Motivation & Goals

- TCAD simulation of 4H-SiC easy
  - create device and run tool

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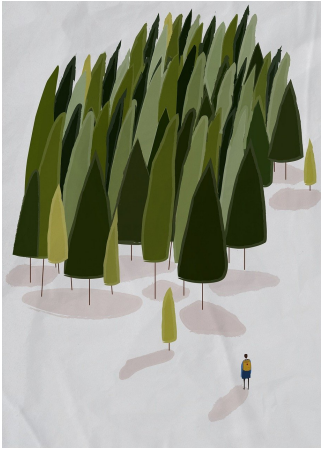
  - contradicting descriptions
  - anisotropies



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  - create device and run tool
- proper model and parameter selection is challenging
  - long history of investigations
  - contradicting descriptions
  - anisotropies
- goals
  - entrance point for newcomers
  - enable scientifically based decision
  - highlight avenues of future research

Research Methods

- theoretical background
  - utilized models and availability in TCAD tools
  - highlight pitfalls

Band Gap: E_{x} denotes both the *free* and *bound* exciton binding energy.

Permittivity: Although $\varepsilon_{\mathrm{s}} = \varepsilon'(\omega \to 0)$ we also found $\varepsilon_{\infty} = \varepsilon'(0)$.

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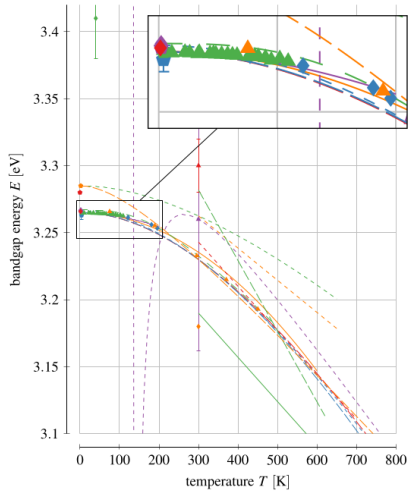
- fundamental publications
  - list achieved model parameters
  - generate comparative plots



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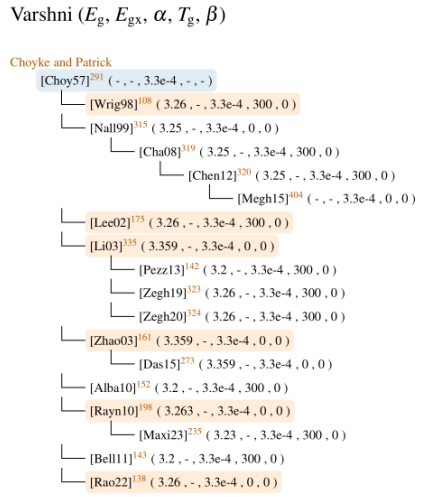
- reference chain
  - show correlations
  - run consistency checks



Research Methods

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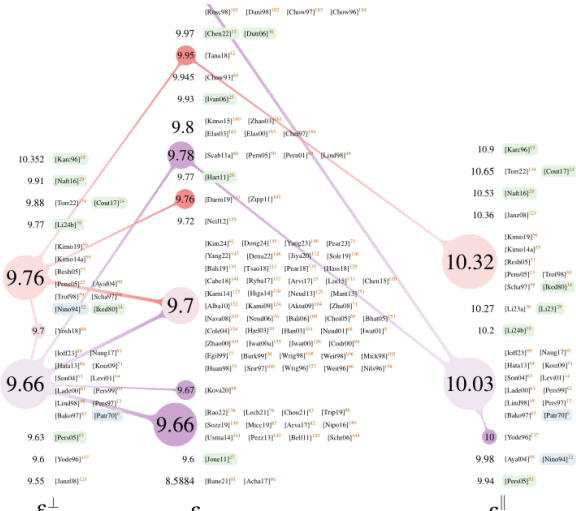
- reference chain
  - show correlations
  - run consistency checks
- parameter overview
  - utilized values within community

Status

- data analysis for topics
  - ✓ relative permittivity (24/10/07)
  - ✓ density-of-states mass (24/10/21)
  - ✓ band gap (24/11/11)
  - ✓ impact ionization (24/10/07)
  - ✓ incomplete ionization (24/10/21)
  - charge carrier recombination
  - mobility
- most recent version available at arXiv:2410.06798

Relative Permittivity

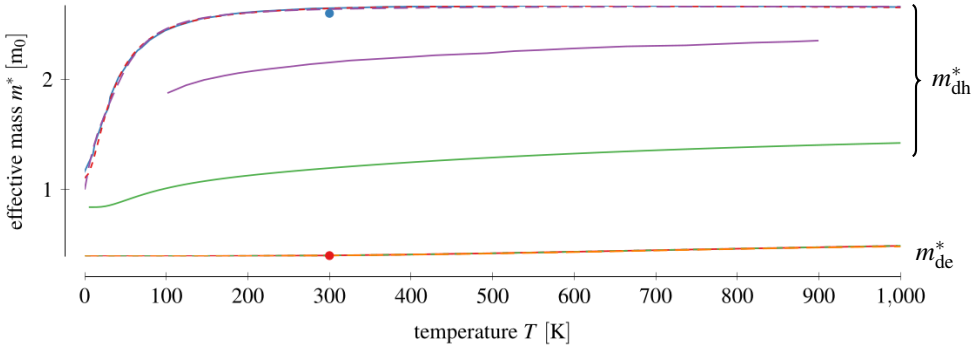
- static (ε_s) and high-frequency (ε_∞) permittivity
  - relative to vaccum permittivity
- most influential publications
  - [Patr70]: based on 6H measurements (1944)
  - [Iked80]: based on 4H measurements (1971)
- values changed over time
  - $9.66 \rightarrow 9.7 \rightarrow 10$
- newer investigations rarely cited
  - long citation chains



Density-of-States Mass

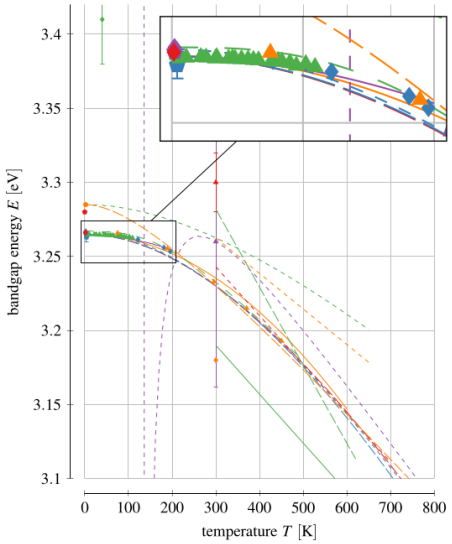
- deviating masses along principal directions
  - $m_d^* = (m_{\perp 1}^* m_{\perp 2}^* m_{\parallel}^*)^{1/3}$
- two conduction bands, three valence bands

- $m_{\mathrm{de}}^* < m_{\mathrm{dh}}^*$
- calculations dominate (0 K)
  - significant $m_{\mathrm{dh}}^*(T)$ often not considered



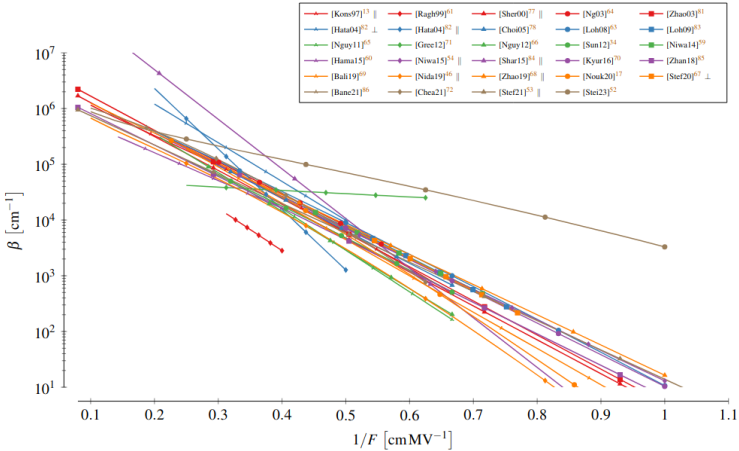
Band Gap

- $E_\mathrm{g} = E_\mathrm{gx} + E_\mathrm{x}$
  - doping and temperature induced narrowing
  - models agree qualitatively
- almost all measurements below $5\,\mathrm{K}$
  - at room temperature large uncertainties
- values changed over time
  - $E_\mathrm{gx} = 3.265\,\mathrm{eV} \rightarrow E_\mathrm{g} = 3.26\,\mathrm{eV}$
- data suggest that $E_\mathrm{g} \approx 3.26\,\mathrm{eV}$
  - verification required



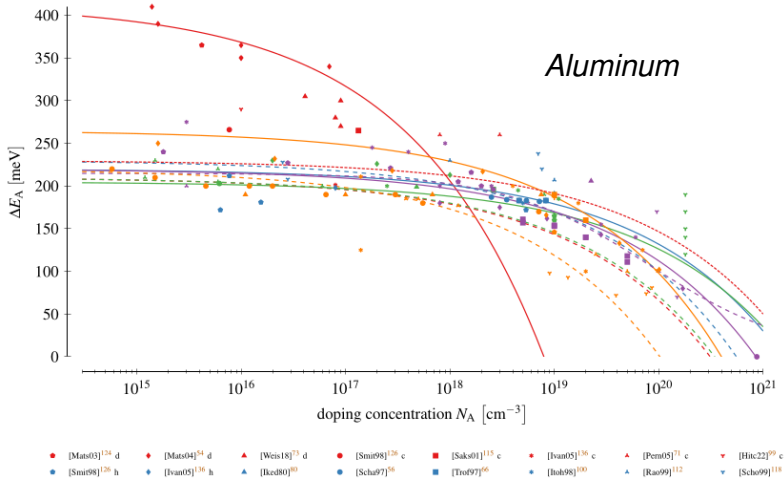
Impact Ionization

- impact ionization coefficients
  - β (holes) $> \alpha$ (electrons)
- no anisotropy for holes
  - $\alpha_\perp > \alpha_\parallel$
- models qualitatively agree for electric field dependency
- β decreases with increasing temperature
  - increase of α reported



Incomplete Ionization

- due to wide band gap not all dopants ionized
  - cubic vs. hexagonal lattice site
- ionization energy decreases with doping concentration
  - novel approaches identified (not in TCAD tools yet)
- Al, B, P, N
  - discussion for higher Aluminum levels



6) Charge Carrier Recombination

Charge Carrier Recombination

- recombination rate R depends on excess charger carrier concentration Δ_N

$$R = R_{\mathrm{SRH}} + R_{\mathrm{bim}} + R_{\mathrm{Auger}} = \frac{\Delta_N}{\tau_{\mathrm{SRH}}} + \frac{\Delta_N}{\tau_{\mathrm{bim}}} + \frac{\Delta_N}{\tau_{\mathrm{Auger}}}$$

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- Shockley-Read-Hall recombination
  - trap assisted recombination
  - bulk and surface contribution
  - doping and temperature dependency

$$R^{\mathrm{b}}_{\mathrm{SRH}} = \frac{np - n_{\mathrm{i}}^2}{\tau_{\mathrm{p}}(n + n_1) + \tau_{\mathrm{n}}(p + p_1)}$$

$$\tau_{\mathrm{n,p}} = (\sigma_{\mathrm{n,p}} v_{\mathrm{th}} N_{\mathrm{t}})^{-1}$$

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- bimolecular recombination
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- bimolecular recombination
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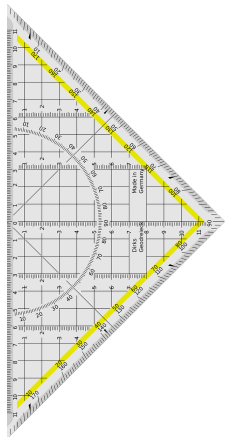
$$R_{\mathrm{bim}} = B(np - n_{\mathrm{i}}^2)$$

- Auger recombination
  - excessive energy to third particle

$$R_{\mathrm{Auger}} = (C_{\mathrm{n}} n + C_{\mathrm{p}} p)(np - n_{\mathrm{i}}^2)$$

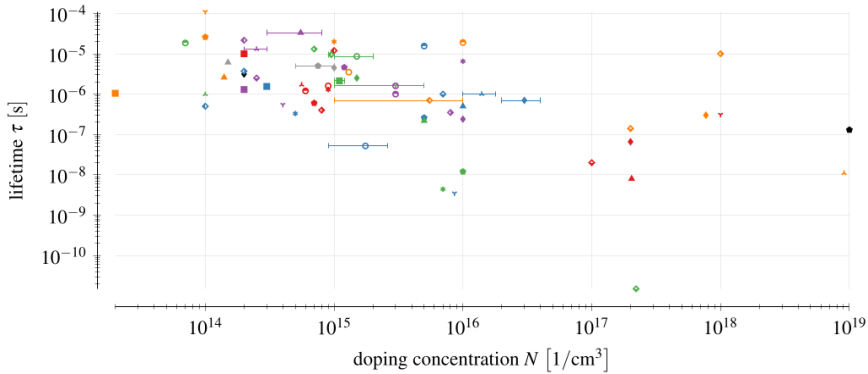
Analysis & Measurements

- $(np - n_i^2) < 0$
  - recombination turns to generation
  - disabled for $R_{\mathrm{bim}} \rightarrow$ optical generation
  - can be activated in some tools for Auger $\rightarrow$ NOT impact ionization
- optical and electrical measurements used
- extracted lifetimes depend on methods and injection level
  - $\tau_{\mathrm{SRH}}^{\mathrm{ll}} = \tau_{\mathrm{n}}$ resp. τ_{p}
  - $\tau_{\mathrm{SRH}}^{\mathrm{hl}} = \tau_{\mathrm{n}} + \tau_{\mathrm{p}}$



SRH Lifetime

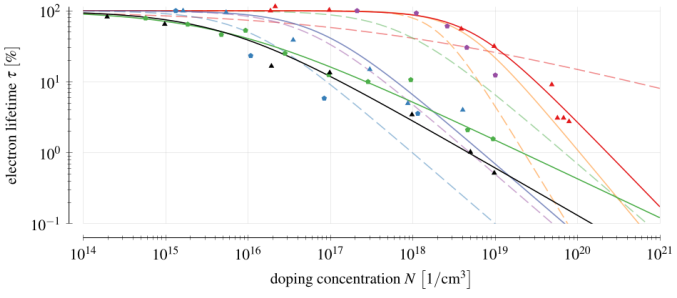
- low ns to one hundred µs (depends on injection level)
- no clear tendency over time



τ_n: red → black, τ_p: blue → green → purple → orange

SRH Lifetime cont'd

- doping induced lifetime reduction
  - measurements suggest deviations among dopants
- most commonly Silicon based model (— —) used
- fit to excess carrier concentration (— —, — —)



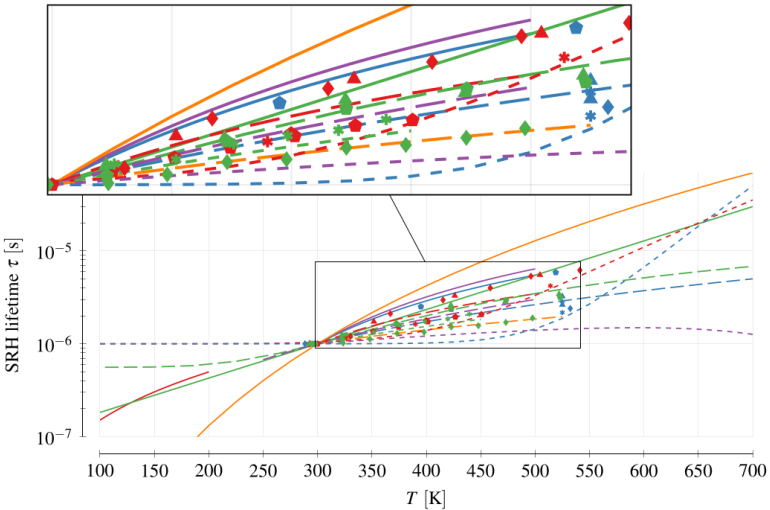
Scharfetter $\underbrace{(N_{\mathrm{ref}}, \gamma)}_{\text{electron}}$ $\underbrace{(N_{\mathrm{ref}}, \gamma)}_{\text{hole}}$

Ruff, Mitlehner, and Helbig

- [Ruff94][227] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Shah98][297] (3×10^{17} , 1) (3×10^{17} , 1)
  - [Lade00][141] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Li03][146] (3×10^{17} , 0.3) (– , –)
    - [Joha16][324] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Zhao03][298] (3×10^{17} , 0.3) (– , –)
  - [Ayal04][64] (6×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Schr06][296] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Buon10][253] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Zhan10][208] (3×10^{17} , 0.3) (– , –)
  - [Buon12][76] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Usma12][307] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
    - [Usma14][204] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
      - [Liu21][323] (3×10^{17} , 1) (3×10^{17} , 1)
  - [Hata13][105] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Das15][312] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Arva17][52] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Hase17][288] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Loph18][151] (1×10^{17} , 0.3) (1×10^{17} , 0.3)
  - [Zhan18][356] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Kaka20][326] (3×10^{17} , 0.3) (3×10^{17} , 0.3)
  - [Koya20][291] (3×10^{17} , 0.3) (3×10^{17} , 0.3)

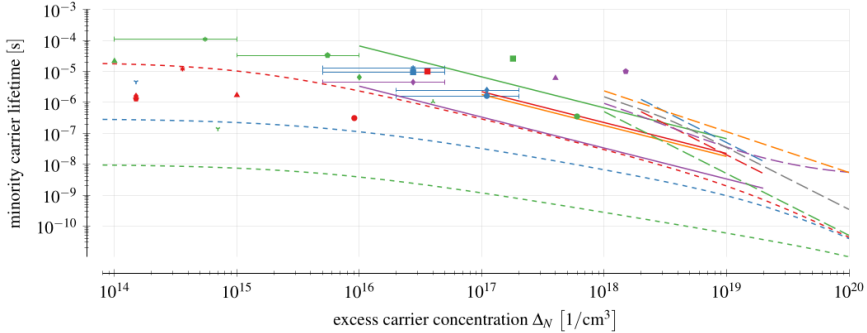
SRH Lifetime cont'd

- increased lifetime with increasing temperature
- most common model (—) only characterized up to 200 K



Combined Lifetime

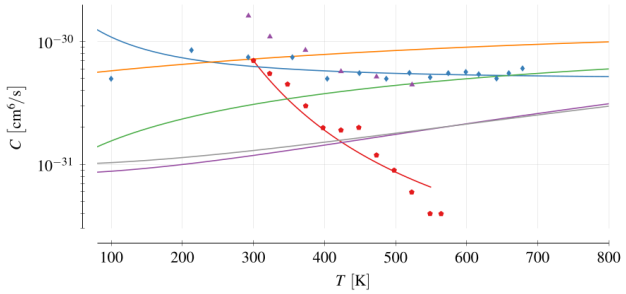
- impact of bimolecular and Auger recombination depends on τ_{SRH}
- parameters only cause vertical shift in log-log space
  - bimolecular slope: -1, Auger slope: -2



τ_{n}: red, τ_{p}: blue $\rightarrow$ green $\rightarrow$ purple

Auger Recombination

- one investigation dominates coefficients
- reduction with temperature observed
  - Silicon based models (—/ —/ —/ —) predict opposite trend



Galeckas *et al.*

- [Gale97][12] ($(5\pm1)\times10^{-31}$, $(2\pm1)\times10^{-31}$, $(7\pm1)\times10^{-31}$, 300)
  - [Gale98][225] ($(5\pm1)\times10^{-31}$, – , $(7\pm1)\times10^{-31}$, 300)
    - [Das15][312] (5×10^{-31} , 9.90×10^{-32} , – , –)
- [Gale99a][46] (– , – , 7×10^{-31} , –)
- [Levi01][143] (5×10^{-31} , 2×10^{-31} , 7×10^{-31} , –)
- [Lee02][220] (5×10^{-31} , 2×10^{-31} , – , –)
- [Neim06][3] (5×10^{-31} , 2×10^{-31} , 7×10^{-31} , –)
- [Alba10][13] (5×10^{-31} , 2×10^{-31} , – , –)
- [Nawa10][162] (5×10^{-31} , 2×10^{-31} , – , –)
- [Habi11][317] (5×10^{-31} , 2×10^{-31} , – , –)
- [Haya11][1] (5×10^{-31} , 2×10^{-31} , – , –)
- [Buon12][76] (5×10^{-31} , 2×10^{-31} , – , –)
- [Pezz13][178] (5×10^{-31} , 2×10^{-31} , – , –)
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  - [Joha19][124] (5×10^{-31} , 2×10^{-31} , – , –)
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- [Kimo18][128] (5×10^{-31} , 2×10^{-31} , – , –)
  - [Chou21][330] (5×10^{-31} , 2×10^{-31} , – , –)
- [Zegh19][119] (5×10^{-31} , 2×10^{-31} , – , –)
- [Tian20][302] (5×10^{-31} , 2×10^{-31} , – , –)
- [Zegh20][118] (5×10^{-31} , 2×10^{-31} , – , –)
- [Asad21][229] (5×10^{-31} , 2×10^{-31} , – , –)
- [Mura21][226] (5×10^{-31} , 2×10^{-31} , – , –)
- [Ioff23][116] (5×10^{-31} , 2×10^{-31} , 7×10^{-31} , –)

Conclusion & Outlook

- review of 4H-SiC TCAD parameters
  - over 1000 publication investigated
  - data analysis for 6 of 7 chapters finished
  - newest results on charge carrier recombination
- latest version available at arXiv:2410.06798
- outlook
  - next up: mobility
  - improve presentation and analyses

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Thank you for your attention.

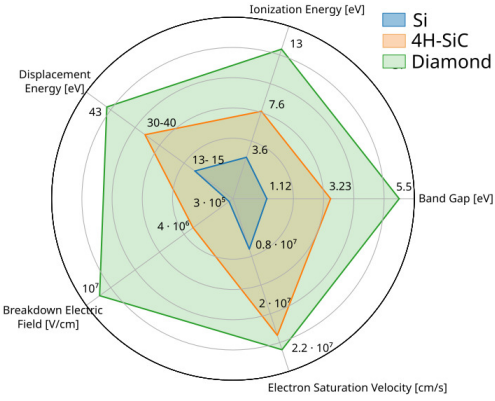
ÖAW AUSTRIAN ACADEMY OF SCIENCES

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS

Backup

Silicon Carbide

- wide bandgap material (WBM)
  - one of first investigated semiconductors
  - used in power electronics
  - polytype 4H commonly used
- features high
  - charge carrier mobilities
  - breakdown field
  - thermal conductance
- utilization @ HEPHY
  - low noise particle detector
  - medical and HEP applications



1) Relative Permittivity

Theory

- TCAD tools use relative permittivity $\varepsilon_\mathrm{r} = \varepsilon/\varepsilon_0$
- complex relative permittivity

$$\varepsilon_\mathrm{r}^*(\omega) = \varepsilon'(\omega) + \mathrm{i}\varepsilon''(\omega)$$

- static relative permittivity $\varepsilon_\mathrm{s} = \varepsilon'(\omega \to 0)$
- high-frequency resp. optical relative permittivity
  - ε' at the end of the reststrahlen range towards higher frequencies, where the real part of the refractive index is null doi:10.1109/EFTF-IFC.2013.6702081
- Lyddane-Sachs-Teller relationship

$$\frac{\varepsilon_\mathrm{s}}{\varepsilon_\infty} = \left(\frac{\omega_{LO}}{\omega_{TO}}\right)^2$$

Caution

- $\varepsilon_s = \varepsilon'(\omega \to 0)$ but sometimes $\varepsilon_\infty = \varepsilon'(0)$
- quote from Patrick *et al.* (1970) doi:10.1103/PhysRevB.2.2255

> *"We shall use ε_∞ to denote the extrapolation … to zero frequency. This somewhat contradictory notation arose because ε_∞ the "optical" dielectric constant, was often set … at a frequency much higher than the lattice frequency, but low compared with electronic transition frequencies. In many substances no suitable frequency exists, and it is preferable to extrapolate optical data to zero frequency …"*

Results

- many fundamental investigations identified
  - measurements and calculations
  - still active field of research

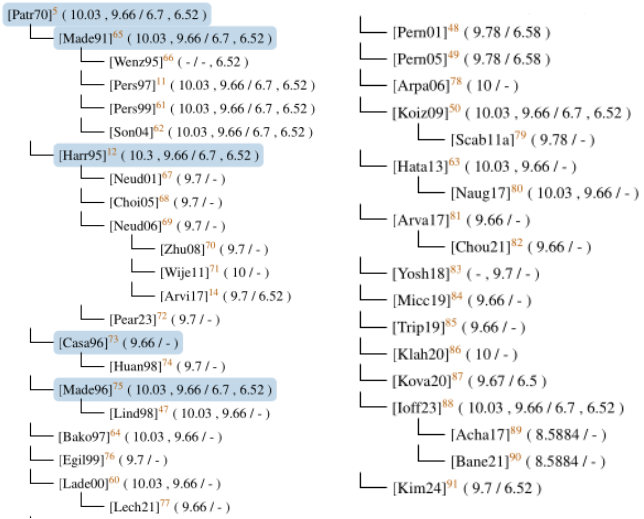
- $\varepsilon_s^{\parallel} > \varepsilon_s^{\perp}$, $\varepsilon_\infty^{\parallel} > \varepsilon_\infty^{\perp}$
- early investigations on 6H
  - based on data from 1940's

ref.	ε_s	$\varepsilon_s^{\parallel}$	$\varepsilon_s^{\perp}$	ε_∞	$\varepsilon_\infty^{\parallel}$	$\varepsilon_\infty^{\perp}$	method[a]	SiC	doping
[Patr70][5]	9.78[c]	10.03	9.66	6.58[c]	6.7	6.52	RI	6H	-
[Iked80][33]	9.94[c]	10.32	9.76	-	-	-	RI	4H	-
[Nino94][31]	9.83[c]	9.98	9.76	6.62[c]	6.67	6.59	SE	6H	-
[Hari95][15]	-	-	-	6.63[c]	6.78	6.56	RI	4H	-
[Karc96][18]	10.53[c]	10.9	10.352	7.02[c]	7.169	6.946	DFT-LDA	4H	-
[Well96][19]	-	-	-	7.02[c]	7.17	6.95	DFT-LDA	4H	-

Note: only first entries shown here

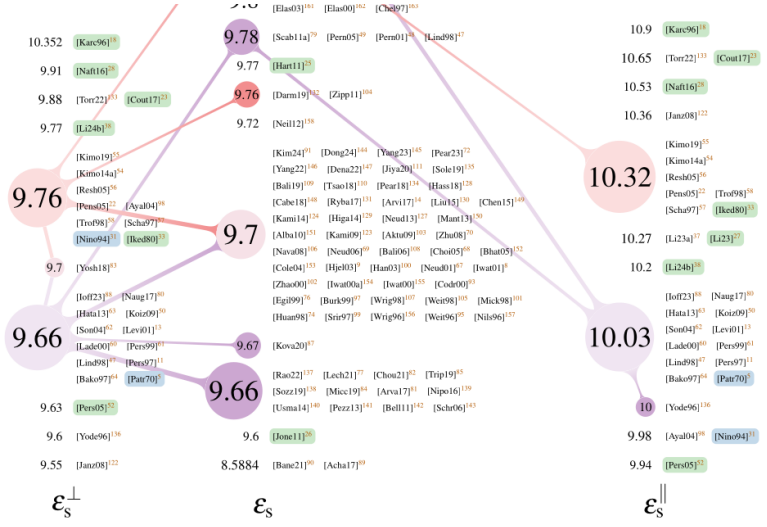
Results cont'd

- 6H values broadly used
  - remarks only in first publications
  - often stated that no 4H values available (until today)
- more recent values are almost not cited at all



Static Permittivity Values

- many values found in literature
  - rounding
  - typographical mistakes
- hard to determine origin
  - found relationships shown in figure



2) Impact Ionization

Theory

- high energy charge carriers create electron-hole pair

$$G_{II} = \frac{1}{q}\left(\alpha J_{\mathrm{n}} + \beta J_{\mathrm{p}}\right) = \frac{1}{q}\left(\alpha n v_n + \beta p v_p\right)$$

- impact ionization coefficients [cm^{-1}]
  - β (holes) $>$ α (electrons) [1, 2]

$$\alpha = \frac{1}{n}\frac{\mathrm{d}n}{\mathrm{d}x}\mathrm{cm}^{-1} \quad , \quad \beta = \frac{1}{p}\frac{\mathrm{d}p}{\mathrm{d}x}\mathrm{cm}^{-1}$$

Empirical Models

Chynoweth's law [3, 4]
Van Overstraeten-de Man [5]

$$\alpha, \beta(F) = a \, \exp\left[-\frac{b}{F}\right]$$

Okuto-Crowell [6]

$$\alpha, \beta(F) = a\{1 + c(T - 300)\} \, F^n \exp\left[-\left(\frac{b\{1 + d(T - 300)\}}{F}\right)^m\right]$$

deviating temperature scaling
$a \to a\gamma$, $b \to b\gamma$

$$\gamma = \frac{\tanh\left(\frac{\hbar\omega_{\mathrm{OP}}}{2k_{\mathrm{B}}T_0}\right)}{\tanh\left(\frac{\hbar\omega_{\mathrm{OP}}}{2k_{\mathrm{B}}T_{\mathrm{L}}}\right)}$$

F ... electric field [V cm^{-1}]

Physics Based Models

Shockley [7]
"lucky electron", low field

$$\alpha, \beta(F) = \frac{eF}{E_\mathrm{i}} \exp\left[-\frac{E_\mathrm{i}}{eF\lambda}\right]$$

Wolff [8]
high field

$$\alpha, \beta(F) = \frac{eF}{E_\mathrm{i}} \exp\left[-\frac{3E_\mathrm{p}E_\mathrm{i}}{(eF\lambda)^2}\right]$$

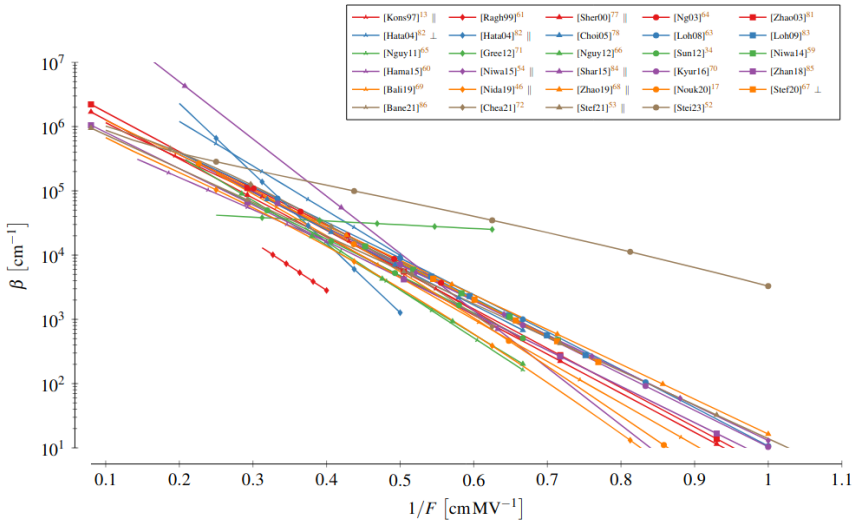
Thornber [9]
arbitrary band structures

$$\alpha, \beta(F) = \frac{eF}{\langle E_\mathrm{i}\rangle} \exp\left[-\frac{\langle E_\mathrm{i}\rangle}{[(eF\lambda)^2/3E_\mathrm{p}] + eF\lambda + E_{k_\mathrm{B}T}}\right]$$

e ... elementary charge, E_i ... ionization energy
λ ... mean free path, E_p ... optical phonon energy, $E_{k_\mathrm{B}T}$ ... thermic phonon energy

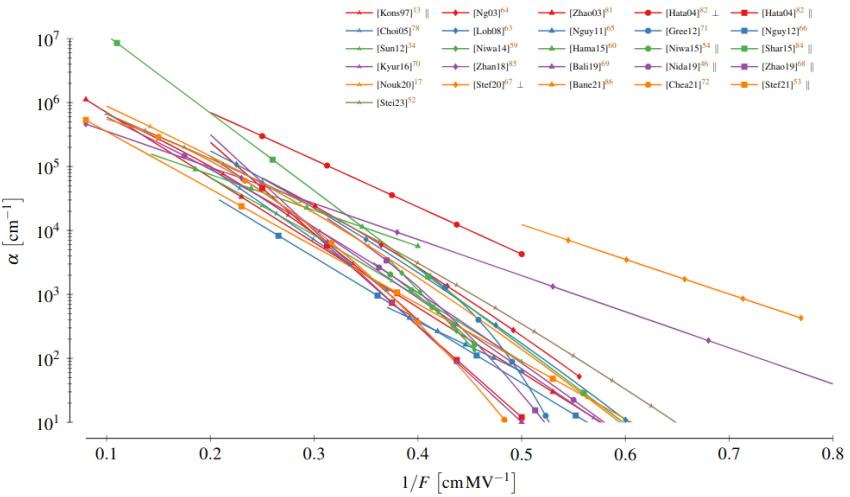
Results Holes

- models only shown where characterized
- good agreement among models
- same results ‖ and ⊥ to c-axis



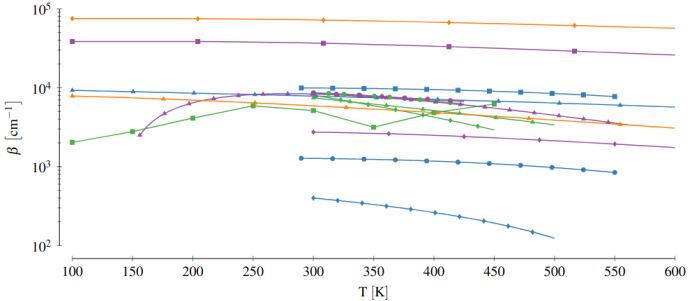
Results Electrons

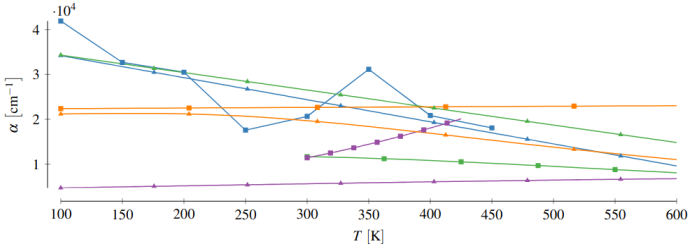
- impact ionization coefficient lower than β
- less agreement among models
- $\perp > \parallel$ to c-axis
- $\perp$: few results



Results Temperature

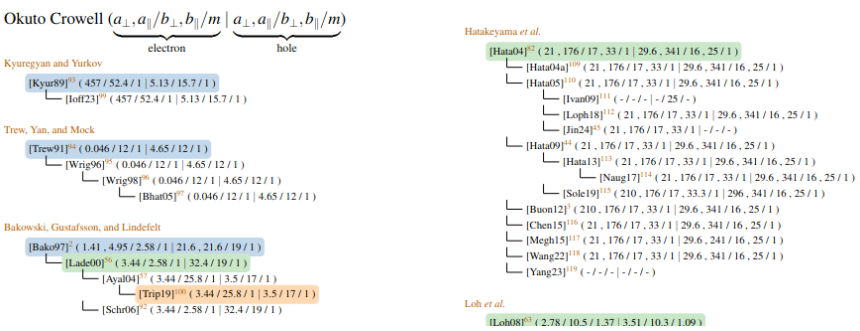
- β decreases with increasing temperature
- increasing α reported
  - compensated by hole temperature dependency
  - $\Delta\alpha < \Delta\beta$
- few investigations
  - most of them in last decade





Insights

- early publications based on 6H values
- most influential publications by Raghunathan *et al.* and Hatakeyama *et al.*



Note: only first entries shown here

3) Incomplete Ionization

Modeling

- due to wide bandgap not all dopants ionized
  - g_A, g_D ... degeneracy factors, new development: $G_A(T)$, $G_D(T)$

$$N_\mathrm{D}^+ = \frac{N_\mathrm{D}}{1 + g_\mathrm{D} \exp\left(\frac{E_\mathrm{F,n} - E_\mathrm{D}}{k_\mathrm{B}T}\right)}, \qquad N_\mathrm{A}^- = \frac{N_\mathrm{A}}{1 + g_\mathrm{A} \exp\left(\frac{E_\mathrm{A} - E_\mathrm{F,p}}{k_\mathrm{B}T}\right)}$$

- in TCAD tools representation using charge carriers beneficial

$$N_\mathrm{D}^+ = \frac{N_\mathrm{D}}{1 + g_\mathrm{D} \frac{n}{N_\mathrm{C}} \exp\left(\frac{\Delta E_\mathrm{D}}{k_\mathrm{B}T}\right)}, \qquad n = N_\mathrm{C} \exp\left(\frac{E_\mathrm{F,n} - E_\mathrm{C}}{k_\mathrm{B}T}\right)$$

$$N_\mathrm{A}^- = \frac{N_\mathrm{A}}{1 + g_\mathrm{A} \frac{p}{N_\mathrm{V}} \exp\left(\frac{\Delta E_\mathrm{A}}{k_\mathrm{B}T}\right)}, \qquad p = N_\mathrm{V} \exp\left(\frac{E_\mathrm{V} - E_\mathrm{F,p}}{k_\mathrm{B}T}\right)$$

Lattice sites

- in general ionization energies differs among hexagonal/cubic lattice sites
- possible to merge to effective ionization energy
  - accuracy degrades

$$N_{\mathrm{D}}^{+} = \frac{\frac{1}{2}N_{\mathrm{D}}}{1 + g_{\mathrm{D}}\frac{p}{N_{\mathrm{C}}}\left(\frac{\Delta E_{\mathrm{Dh}}}{k_{\mathrm{B}}T}\right)} + \frac{\frac{1}{2}N_{\mathrm{D}}}{1 + g_{\mathrm{D}}\frac{p}{N_{\mathrm{C}}}\left(\frac{\Delta E_{\mathrm{Dc}}}{k_{\mathrm{B}}T}\right)}$$

$$N_{\mathrm{A}}^{-} = \frac{\frac{1}{2}N_{\mathrm{A}}}{1 + g_{\mathrm{A}}\frac{p}{N_{\mathrm{V}}}\left(\frac{\Delta E_{\mathrm{Ah}}}{k_{\mathrm{B}}T}\right)} + \frac{\frac{1}{2}N_{\mathrm{A}}}{1 + g_{\mathrm{A}}\frac{p}{N_{\mathrm{V}}}\left(\frac{\Delta E_{\mathrm{Ac}}}{k_{\mathrm{B}}T}\right)}$$

$E_{\mathrm{Dc}}, E_{\mathrm{Dh}} \ldots$ cubic/hexagonal donor ionization energy

$E_{\mathrm{Ac}}, E_{\mathrm{Ah}} \ldots$ cubic/hexagonal acceptor ionization energy

Doping Dependency

- ionization energy depends on doping
  - changing potential energy of charge carriers when closer to ionized atoms

$$\Delta E(N) = \Delta E_0 - \alpha N^{1/3}$$

- $N \gg 0 \rightarrow \Delta E < 0$
  - not possible since screening dominant effect
  - logistic equation fitting prevents that (not in TCAD tools yet)

$$\Delta E(N) = \frac{\Delta E_0}{1 + (N/N_{\mathrm{E}})^c}$$

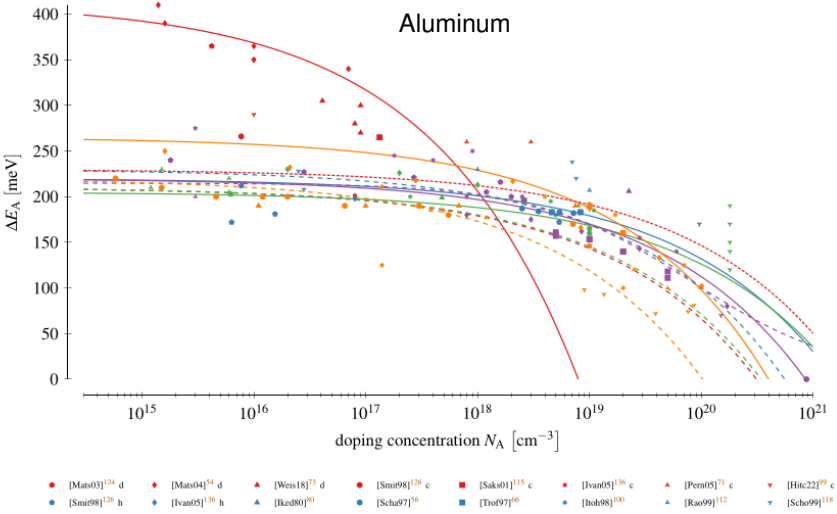
Characterization Methods

- Hall measurements
  - neutrality equation
  - activation ratio
  - free carrier concentration spectroscopy
- other electrical measurements
  - (thermal) admittance spectroscopy
  - electron spin resonance
  - deep level transient spectroscopy
  - minority carrier transient spectroscopy
- fitting to existing data

- optical measurements
  - photothermal ionizatoin spectroscopy
  - donor-acceptor pair luminescence
  - time-resolved spectroscopy
  - delay measurements
- calculations
  - Faulkner model
  - density functional theory
  - effective mass approximation
  - first principle
  - *ab initio* supercell

Results

- Aluminum
  - lots of data
- Boron
  - confused with D-center
- Nitrogen
  - no energy loss for cubic site
- Phosphorus
  - little data available



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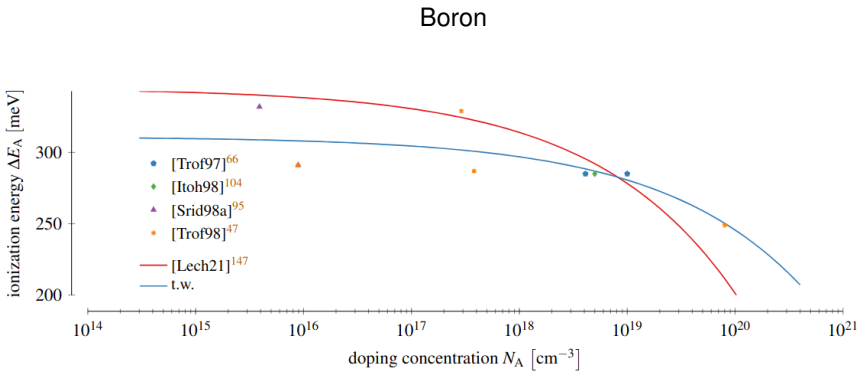

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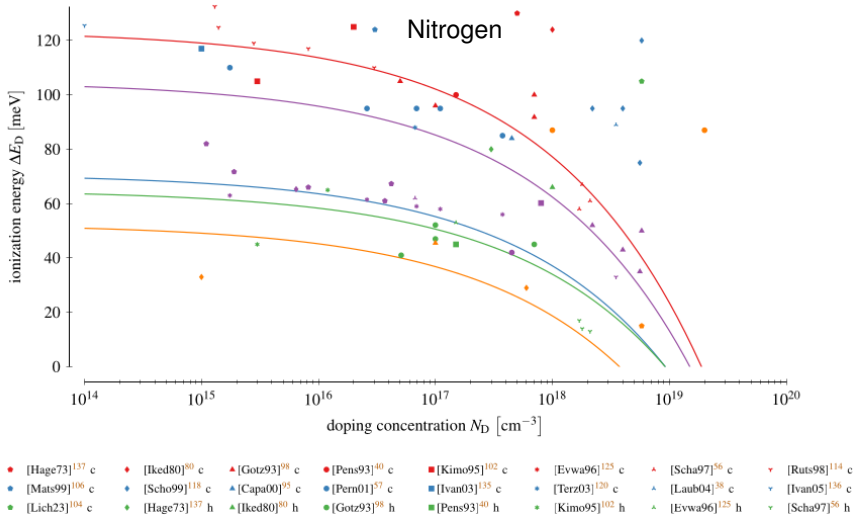

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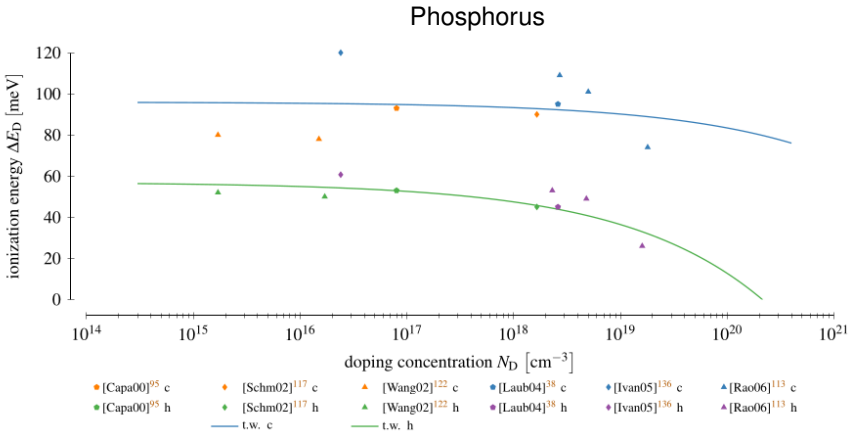
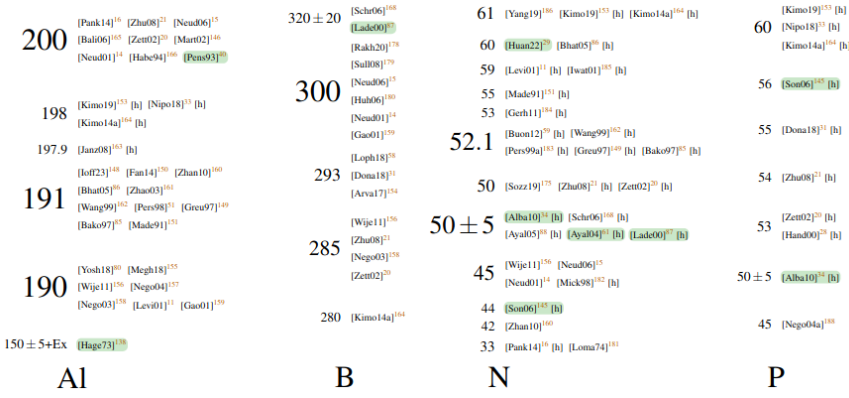


Additional Analyses

- charge carrier cross sections
- reference chains and value consistency
- single ionization energy values



Note: only first entries shown here

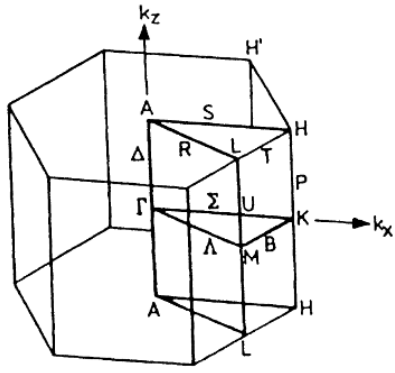
4) Density-of-States Mass

Effective Mass

- mass a charge carrier seems to have on interactions
- in TCAD often used
  - density-of-states mass
  - conductivity mass
  - tunneling mass
  - quantum well mass
  - at contact or in a channel
- focus of review
  - density-of-states mass
  - shortly conductivity mass

Principal Directions

- effective mass expressed in multiples of free electron mass m_0
- electrons
  - conduction band minimum in M-point
  - $\parallel$ to c-axis: m^*_{ML}
  - $\perp$ to c-axis: $m^*_{\mathrm{M\Gamma}}, m^*_{\mathrm{MK}}$
- holes
  - valence band maximum in Γ-point
  - $\parallel$ to c-axis: $m^*_{\Gamma\mathrm{A}}$
  - $\perp$ to c-axis: $m^*_{\Gamma\mathrm{M}}, m^*_{\Gamma\mathrm{K}}$



[Käckell1994] doi:10.1103/PhysRevB.50.10761

Density-of-States (DOS) Mass

- density of states for conduction (N_C) and valence (N_V) band
  - $M_C \ldots$ number of conduction band minima in the first Brillouin zone

$$N_C = 2\,M_C \left(\frac{2\pi m^*_{de} k_B T}{h^2}\right)^{3/2}, \qquad N_V = 2 \left(\frac{2\pi m^*_{dh} k_B T}{h^2}\right)^{3/2}$$

- effective masses for electrons (m^*_{de}) and holes (m^*_{dh})

$$m^*_{de} = (m^*_{de\perp}{}^2 m^*_{de\parallel})^{1/3} = (m^*_{M\Gamma} m^*_{MK} m^*_{ML})^{1/3}, \qquad m^*_{dh} = (m^*_{dh\perp}{}^2 m^*_{dh\parallel})^{1/3} = (m^*_{\Gamma M} m^*_{\Gamma K} m^*_{\Gamma A})^{1/3}$$

DOS Mass cont'd

- combine two topmost valence bands …

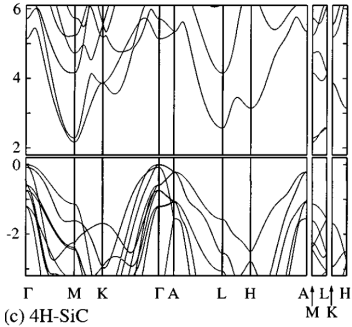
$$m^*_{\mathrm{dh}} = \left({m^*_{\mathrm{hh}}}^{3/2} + {m^*_{\mathrm{lh}}}^{3/2} \right)^{2/3} .$$

- … or even all three

$$m^*_{\mathrm{h}}(T) = \left[m_{\mathrm{h1}}^{3/2} + m_{\mathrm{h2}}^{3/2} \exp\left(-\frac{\Delta E_2}{k_{\mathrm{B}} T} \right) + m_{\mathrm{h3}}^{3/2} \exp\left(-\frac{\Delta E_3}{k_{\mathrm{B}} T} \right) \right]^{2/3}$$

- temperature dependency

$$m^*(T) = \left(\frac{z_0 + z_1 T + z_2 T^2 + z_3 T^3 + z_4 T^4}{1 + n_1 T + n_2 T^2 + n_3 T^3 + n_4 T^4} \right)^{\eta}$$



(c) 4H-SiC

[Persson1997] doi:10.1063/1.365578

Polaron Mass

- carbon atoms more electronegative in Si-C bond
  - optical vibrations generate electric field → slightly increased *polaron mass*

$$m_\mathrm{p} = m\frac{1-8\times10^{-4}\alpha^2}{1-\alpha/6+3.4\times10^{-3}\alpha^2} \approx m\left(1-\frac{\alpha}{6}\right)^{-1}$$

- Fröhlich constant α
  - term $1/4\pi\varepsilon_\mathrm{s}$ missing in some publications (differing unit system)

$$\alpha = \frac{1}{2}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_\mathrm{s}}\right)\frac{e^2}{\hbar\omega_\mathrm{LO}}\left(\frac{2m\omega_\mathrm{LO}}{\hbar}\right)^{1/2}\frac{1}{4\pi\varepsilon_\mathrm{s}}$$

$\varepsilon_\mathrm{s}/\varepsilon_\infty$ … static/high-frequency dielectric constant

ω_LO … longitudinal optical phonon frequency

Characterization Methods

- density functional theory local density approximation (DFT-LDA) calculations
  - projector augmented wave
  - (full-potential) linearized augmented plane wave
  - orthogonalized) linear combination of atomic orbital
  - full-potential linear muffin-tin orbital
  - hybrid pseudo-potential and tight-binding
- other calculations
  - empirical pseudo potentials
  - RSP Hamiltonians
- Monte Carlo simulations
- measurements
  - optically detected cyclotron resonance
  - photoluminescence
  - infrared absorption
  - Raman scattering
  - Hall effect
- fitting
  - genetic algorithm
  - gradual parameter refinement

Results Principal Directions

- data for all bands available
  - mostly from 1994-2004
- heavily based on calculations
  - two measurements for electrons, none for holes

	electron				hole					
ref.	m^*_{MI} [m_0]	m^*_{MK} [m_0]	m^*_{ML} [m_0]	band	m^*_{TM} [m_0]	m^*_{TK} [m_0]	m^*_{TA} [m_0]	band	method[a]	polaron
[Kack94][54]	0.62	0.13	0.39	-	4.23	2.41	1.73	hh	DFT-LDA	-
	-	-	-	-	0.45	0.77	1.73	lh	DFT-LDA	-
	-	-	-	-	0.74	0.51	0.21	so	DFT-LDA	-
[Karc95][16]	0.66	0.31	0.3	-	-	-	-	-	DFT-LDA	-
[Lamb95][61]	0.58	0.28	0.31	-	-	-	-	-	DFT-LDA	-
[Wenz95][56]	0.6	0.28	0.19	-	-	-	-	-	DFT-LDA	-
[Nils96][55]	0.43	0.43	0.28	1	-	-	-	-	DFT-LDA	-
	0.52	0.21	0.45	2	-	-	-	-	DFT-LDA	-

Note: only first entries shown here

Results DOS Mass

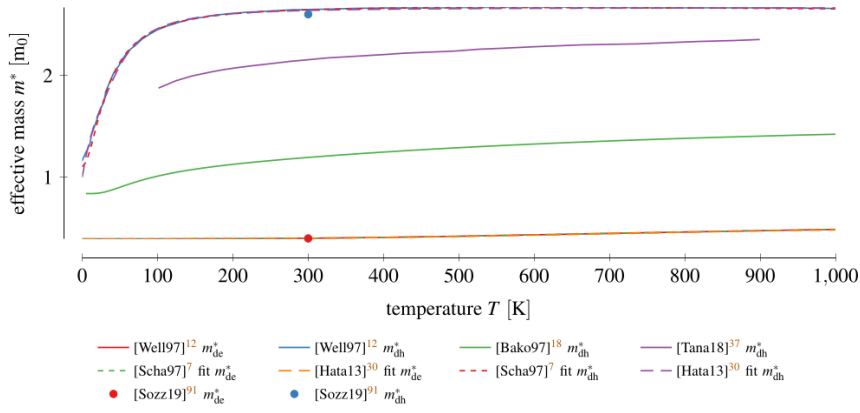
- existing data extended by calculations using masses in principal directions
- more measurement results found
  - still calculations dominant

ref.	electron				hole					
	m^*_{de} [m_0]	$m^*_{de\perp}$ [m_0]	$m^*_{de\parallel}$ [m_0]	band	m^*_{dh} [m_0]	$m^*_{dh\perp}$ [m_0]	$m^*_{dh\parallel}$ [m_0]	band	method[h]	polaron
[Loma73][72]	0.20[a]	0.21	0.19	-	-	-	-	-	Hall	-
[Loma74][73]	0.20[a]	0.21	0.19	-	-	-	-	-	Hall	-
[Gotz93][32]	0.19	0.176	0.224	-	-	-	-	-	IR	-
[Kack94][54]	0.31[a]	0.28[b]	0.39[c]	-	2.60[a]	3.19[b]	1.73[c]	hh	DFT-LDA	-
	-	-	-	-	0.84[a]	0.59[b]	1.73[c]	lh	DFT-LDA	-
	-	-	-	-	0.43[a]	0.61[b]	0.21[c]	so	DFT-LDA	-
[Hari95][70]	0.35[a]	0.30 ± 0.07	0.48 ± 0.12	-	-	-	-	-	Raman	-

Note: only first entries shown here

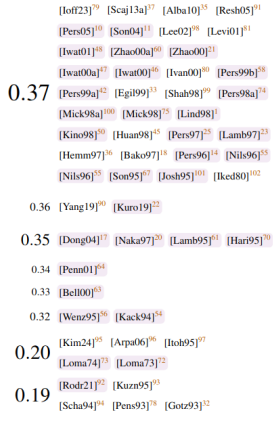
Results Temperature Dependency

- three investigations identified
  - only single one referenced and fitted
- significant change to hole mass
  - most values only valid close to 0 K



Results TCAD values

- wide range of values
  - 0.19 - 0.48 for electrons
  - 0.43 - 2.91 for holes
- temperature barely considered
  - hole mass for room temperature often too low
  - even when considered wrong values stated
- additional analyses
  - miscalculations identified
  - citations and value consistency



Note: only first entries shown here

Conductivity Mass

- required for investigations of mobility

$$\mu = \frac{e\tau}{m_c^*}$$

- effective masses for electrons (m_{ce}^*) and holes (m_{ch}^*)

$$\frac{3}{m_{\mathrm{ce}}^*} = \frac{1}{m_{\mathrm{M\Gamma}}^*} + \frac{1}{m_{\mathrm{MK}}^*} + \frac{1}{m_{\mathrm{ML}}^*}, \qquad \frac{3}{m_{\mathrm{ch}}^*} = \frac{1}{m_{\mathrm{\Gamma M}}^*} + \frac{1}{m_{\mathrm{\Gamma K}}^*} + \frac{1}{m_{\mathrm{\Gamma A}}^*}$$

5) Band Gap

Band Gap Energy

band gap E_g = exciton band gap E_gx + free exciton binding energy E_x

free exciton binding energy

- energy required to free electron from exciton
- E_x

bound exciton binding energy

- amount of exciton energy reduction when attached to impurity
- depends on impurity type
- E_x

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free exciton binding energy

- energy required to free electron from exciton
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bound exciton binding energy

- amount of exciton energy reduction when attached to impurity
- depends on impurity type
- E_x

$$E_\mathrm{g}(T, N_\mathrm{D}^+, N_\mathrm{A}^-) = E_\mathrm{g}(T) - \Delta E_\mathrm{g}(N_\mathrm{D}^+, N_\mathrm{A}^-)$$

Temperature Dependency

- Varshni relation

$$E_g(T) = E_g(T_g) + \alpha \left(\frac{T_g^2}{T_g + \beta} - \frac{T^2}{T + \beta} \right)$$

- Bose-Einstein type

$$E_g(T) = E_B - \alpha_B \left(1 + \frac{2}{e^{\Theta_B/T} - 1} \right)$$

- Pässler model

$$E_g(T) = E_g(0) - \frac{\varepsilon \Theta_p}{2} \left[\sqrt[p]{1 + \left(\frac{2T}{\Theta_p} \right)^p} - 1 \right], \qquad p \approx \sqrt{\frac{1}{\Delta^2} + 1}$$

- $\Delta \ldots$ phonon dispersion ($\Delta > 1 \ldots$ Varshni, $\Delta \to 0 \ldots$ Bose-Einstein)
- $\Theta_p \ldots$ average phonon temperature, $\varepsilon \ldots$ entropy

Doping Dependency

- Lindefelt

$$\Delta E_{\mathrm{g}}(N_{\mathrm{D}}^{+}, N_{\mathrm{A}}^{-}) = -\Delta E_{(\mathrm{n/p})\mathrm{c}}(N_{\mathrm{D}}^{+}) + \Delta E_{(\mathrm{n/p})\mathrm{v}}(N_{\mathrm{A}}^{-})$$

$$\Delta E_{\mathrm{nc}}(N_{\mathrm{D}}^{+}) = A_{\mathrm{nc}} \left(\frac{N_{\mathrm{D}}^{+}}{10^{18}} \right)^{1/3} + B_{\mathrm{nc}} \left(\frac{N_{\mathrm{D}}^{+}}{10^{18}} \right)^{1/2} < 0$$

$$\Delta E_{\mathrm{nv}}(N_{\mathrm{D}}^{+}) = A_{\mathrm{nv}} \left(\frac{N_{\mathrm{D}}^{+}}{10^{18}} \right)^{1/4} + B_{\mathrm{nv}} \left(\frac{N_{\mathrm{D}}^{+}}{10^{18}} \right)^{1/2} > 0$$

$$\Delta E_{\mathrm{pc}}(N_{\mathrm{D}}^{+}) = A_{\mathrm{pc}} \left(\frac{N_{\mathrm{A}}^{-}}{10^{18}} \right)^{1/4} + B_{\mathrm{pc}} \left(\frac{N_{\mathrm{A}}^{-}}{10^{18}} \right)^{1/2} < 0$$

$$\Delta E_{\mathrm{pv}}(N_{\mathrm{D}}^{+}) = A_{\mathrm{pv}} \left(\frac{N_{\mathrm{A}}^{-}}{10^{18}} \right)^{1/3} + B_{\mathrm{pv}} \left(\frac{N_{\mathrm{A}}^{-}}{10^{18}} \right)^{1/2} + C_{\mathrm{pv}} \left(\frac{N_{\mathrm{A}}^{-}}{N_{\mathrm{A0}}} \right)^{1/4} > 0$$

Doping Dependency cont'd

- Slotboom

$$\Delta E_{\mathrm{g}} = C_{\mathrm{n,p}} \left(\ln\left(\frac{N}{N_{\mathrm{n,p}}}\right) + \sqrt{\left(\ln\left(\frac{N}{N_{\mathrm{n,p}}}\right)\right)^2 + G} \right)$$

- Schubert
  - not able to reproduce plots found in literature

$$\Delta E_{\mathrm{g}} = \frac{e^3\sqrt{n}}{4\pi\varepsilon^{3/2}\sqrt{k_{\mathrm{B}}T}} \qquad \text{(Debye, non-degenerate)}$$

$$\Delta E_{\mathrm{g}} = \frac{e^3\sqrt{m^*_{\mathrm{de}}(3n)^{1/3}}}{4\pi^{5/3}\varepsilon^{3/2}\hbar} \qquad \text{(Thomas-Fermi, degenerate)}$$

Characterization Methods

- optical measurements
  - transmission spectroscopy
  - photo absorption
  - optical admittance
  - exciton electroabsorptions
  - free carrier absorption
  - free exciton luminescence
  - photoluminescence
  - photconductivity
  - wavelength-modulated absorption
- calculations
  - empirical pseudopotentials
  - density functional theory
  - rectangular barrier
- fitting to existing data
  - including genetic algorithm

Results

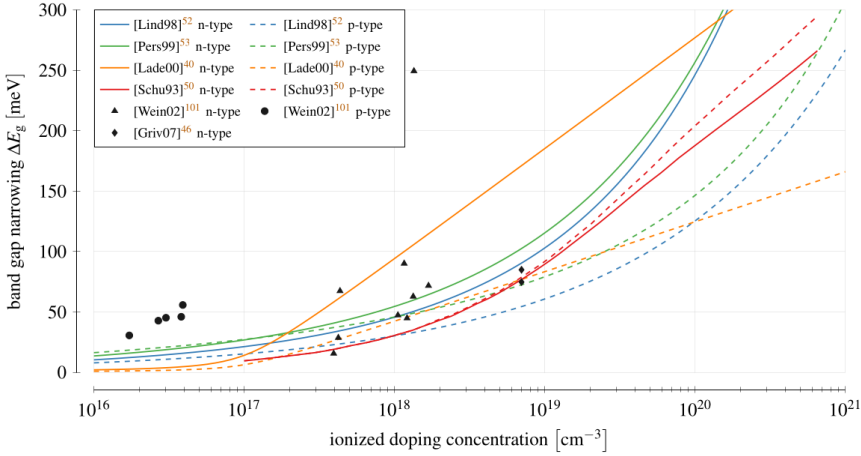
- measurements mainly of E_{gx} at low temperatures
  - $E_{gx} = 3.265(2)$ eV
- latest calculations predict clearly lower values
  - $E_g = 3.15(3)$ eV

ref.	band gap			temperature dep.				
	E_g [eV]	E_{gx} [eV]	E_x [meV]	T_g [K]	α [eV K^{-1}]	β [K]	interval [K]	method[80]
[Choy57][59 81]	-	-	-	-	3.3×10^{-4}	-	-	PA
[Choy64][24]	-	3.263 ± 0.003	-	4	-	-	-	PA
[Choy64a][23 82]	-	3.265	-	4.7	-	-	-	PA
[Jung70][67]	2.8	-	-	0	-	-	-	EP
[Dubr75][20]	-	-	20 ± 15	-	-	-	-	EE

Note: only first entries shown here

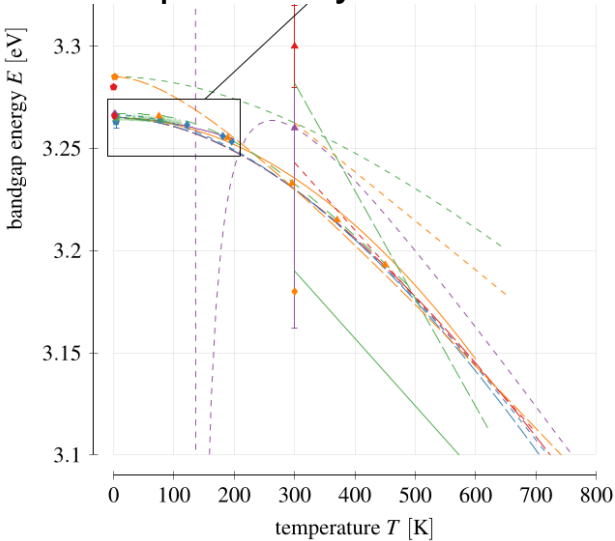
Doping Dependency

- increasing narrowing with doping concentration
- too few measurements to verify



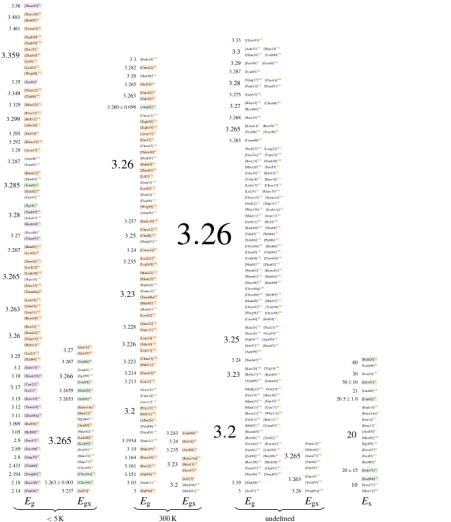
Temperature Dependency

- band gap decreases with temperature
- differences between Varshni and Bose-Einstein barely visible
- almost always separation of E_{g} and E_{gx}
- big uncertainty for room temperature measurements



Band Gap Values

- overwhelming amount of values in literature
  - very few temperature scaling parameters
  - $E_\mathrm{g}(T_\mathrm{g})$ main difference
- analysis results
  - all values go back to measurements of E_gx at low temperature in 1964 (3.263 eV,3.265 eV,3.23 eV)
  - then rounding and $E_\mathrm{gx} \rightarrow E_\mathrm{g}$
  - coincidentally measurement of $E_\mathrm{g}(300) \approx 3.26\,\mathrm{eV}$
- future research
  - room temperature measurements for verification
  - temperature dependency of E_x



6) Charge Carrier Recombination

Characterization Methods

- optical measurements
  - (microwave) photoconductance decay ((μ)-PCD)
  - photoluminescence decay (PLD)
  - (transient) (time-resolved) free carrier absorption ((T)(TR-)FCA)
  - electron beam induced current (EBIC)
  - time-resolved photoinduced absorption (TRPA)
  - time-resolved photoluminescence (TRPL)
  - time-resolved transient absorption (TRTA)
  - transient absorption spectroscopy (TAS)
  - four wave mixing (FWM)
  - low-temperature photoluminescence (LTPL)
  - capacitance transient (C-t)
  - differential transmittivity (DT)
- electrical measurements
  - reverse recovery (RR)
  - thyristor turned off gate current (TTOGC)
  - short-circuit current/open-circuit voltage decay (SCCVD/ OCVD)
  - diode current density (DCD)
  - bipolar transistor emitter current (BTEC)
  - diode forward voltage degradation (DFVD)
- fitting to existing data and simulations

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