



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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- TCAD simulation of 4H-SiC easy
 - create device and run tool
- proper model and parameter selection is challenging
 - long history of investigations
 - contradicting descriptions
 - anisotropies





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Motivation & Goals



- TCAD simulation of 4H-SiC easy
 - 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





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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 $\overline{\varepsilon_s} = \varepsilon'(\omega \to 0)$ we also found $\varepsilon_{\infty} = \varepsilon'(0)$.



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Research Methods



- theoretical background
 - utilized models and availability in TCAD tools
 - highlight pitfalls
- fundamental publications
 - list achieved model parameters
 - generate comparative plots





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Research Methods



Varshni $(E_g, E_{gx}, \alpha, T_g, \beta)$

Choyke and Patrick [Chov57]²⁹¹ (-.-. 3.3e-4.-.-) [Wrig98]¹⁰⁸ (3.26, -, 3.3e-4, 300, 0) - [Nall99]³¹⁵ (3.25, -, 3.3e-4, 0, 0) - [Cha08]³¹⁹ (3.25, -, 3.3e-4, 300, 0) $[Chen 12]^{320}$ (3.25, -, 3.3e-4, 300, 0) [Megh15]⁴⁰⁴ (- . - . 3.3e-4 . 0 . 0) $[Lee02]^{175}$ (3.26, -, 3.3e-4, 300, 0) $[Li03]^{335}$ (3.359, -, 3.3e-4, 0, 0) - [Pezz13]¹⁴² (3.2, -, 3.3e-4, 300, 0) - [Zegh19]³²³ (3.26, -, 3.3e-4, 300, 0) [Zegh20]³²⁴ (3.26, -, 3.3e-4, 300, 0) [Zhao03]¹⁶¹ (3.359, -, 3.3e-4, 0, 0) - [Alba10]¹⁵² (3.2. - . 3.3e-4. 300. 0) [Rayn10]¹⁹⁸ (3.263, -, 3.3e-4, 0, 0) [Bell11]¹⁴³ (3.2 , - , 3.3e-4 , 300 , 0) [Rao221138 (3.26 - 3.3e-4 0.0)

• theoretical background

- utilized models and availability in TCAD tools
- highlight pitfalls
- fundamental publications
 - list achieved model parameters
 - generate comparative plots
- reference chain
 - show correlations
 - run consistency checks





[Levi01b1303

		$ au_{ m n}$		$ au_{ m p}$
 utilized values within community 	I	[Adit15] ²⁶⁷	0.015	[Bell11] ⁷¹
parameter overview	1	[Ioff23] ¹¹⁶	0.05	[Das15] ³¹²
2	.5	[Das15] ³¹²		[Bell09] ³⁰⁴
 run consistency checks 	5	[Cha08] ³¹³	15	[Pezz13]178
- show correlations	8	[Bell11] ⁷¹		[Rao22] ³⁰⁵
	10	[Megh15] ³¹⁴	20	[Ayal04] ⁵⁴
• reference chain		[Bell09] ³⁶⁴		[Schr06] ²⁹⁶
	5	[Pezz13] ¹⁷⁸	50	[Nall99] ²³⁹
		[Rao22] ³⁰⁵	50	[Usma12]***
- list achieved model parameters	40	[Zhao00] ³¹⁵		[Choi05]***
fundamental publications	50	[Nall99] ²¹⁹	100	[Zegh19] ³¹⁹
ing ing it pitalo		[Usma12] ³⁰⁷		[Zegh20] ³¹⁸
 highlight pitfalls 	00	[Ayal04] ⁶⁴	120	[Lech21] ²³⁸
 utilized models and availability in TCAD tools 		[Schr06]296	150	[Nayd21] ³¹⁶
 theoretical background 	50	[Navd21] ³¹⁶	200	[Cha08] ³¹³
26	50	[Habi11] ³¹⁷	260	[Levi01] ¹⁴⁵
30	00	[Levi01b] ³⁰³		

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SCIENCES





- 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







- static ($\epsilon_s)$ and high-frequency ($\epsilon_\infty)$ permittivity
 - relative to vaccum permittivity
- most influential publications

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- [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

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





Band Gap



• $E_{\rm g} = E_{\rm gx} + E_{\rm x}$

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





Impact Ionization



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







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- cubic vs. hexagonal lattice site
- ionization energy decreases with doping concentration
 - novel approaches identified (not in TCAD tools yet)

• AI, B, P, N

- discussion for higher Aluminum levels







6) Charge Carrier Recombination





• recombination rate R depends on excess charger carrier concentration Δ_N

$$R = R_{ ext{SRH}} + R_{ ext{bim}} + R_{ ext{Auger}} = rac{\Delta_N}{ au_{ ext{SRH}}} + rac{\Delta_N}{ au_{ ext{bim}}} + rac{\Delta_N}{ au_{ ext{Auger}}}$$

11

• recombination rate R depends on excess charger carrier concentration Δ_N

$$R = R_{ ext{SRH}} + R_{ ext{bim}} + R_{ ext{Auger}} = rac{\Delta_N}{ au_{ ext{SRH}}} + rac{\Delta_N}{ au_{ ext{bim}}} + rac{\Delta_N}{ au_{ ext{Auger}}}$$

Charge Carrier Recombination

- Shockley-Read-Hall recombination
 - trap assisted recombination

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- bulk and surface contribution
- doping and temperature dependency

 $R_{\rm SRH}^{\rm b} = \frac{np - n_{\rm i}^2}{\tau_{\rm p}(n + n_1) + \tau_{\rm n}(p + p_1)}$ $\tau_{\rm n,p} = (\sigma_{\rm n,p} v_{\rm th} N_{\rm t})^{-1}$



Charge Carrier Recombination

• recombination rate R depends on excess charger carrier concentration Δ_N

$$R = R_{ ext{SRH}} + R_{ ext{bim}} + R_{ ext{Auger}} = rac{\Delta_N}{ au_{ ext{SRH}}} + rac{\Delta_N}{ au_{ ext{bim}}} + rac{\Delta_N}{ au_{ ext{Auger}}}$$

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

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- radiative, DAP, e-A, TAA

$$R_{\text{SRH}}^{\text{b}} = \frac{np - n_{\text{i}}^2}{\tau_{\text{p}}(n+n_1) + \tau_{\text{n}}(p+p_1)}$$
$$\tau_{\text{n},\text{p}} = (\sigma_{\text{n},\text{p}}\nu_{\text{th}}N_{\text{t}})^{-1}$$

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



Charge Carrier Recombination

• recombination rate *R* depends on excess charger carrier concentration Δ_N

$$R = R_{
m SRH} + R_{
m bim} + R_{
m Auger} = rac{\Delta_N}{ au_{
m SRH}} + rac{\Delta_N}{ au_{
m bim}} + rac{\Delta_N}{ au_{
m Auger}}$$

- Shockley-Read-Hall recombination
 - trap assisted recombination
 - bulk and surface contribution
 - doping and temperature dependency
- bimolecular recombination
 - radiative, DAP, e-A, TAA
- Auger recombination

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- excessive energy to third particle

$$R_{\text{SRH}}^{\text{b}} = \frac{np - n_{\text{i}}^2}{\tau_{\text{p}}(n+n_1) + \tau_{\text{n}}(p+p_1)}$$
$$\tau_{\text{n},\text{p}} = (\sigma_{\text{n},p}v_{\text{th}}N_{\text{t}})^{-1}$$

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

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





Analysis & Measurements



• $(np-n_i^2) < 0$

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- recombination turns to generation
- disabled for $R_{
 m bim}
 ightarrow$ optical generation
- can be activated in some tools for $\mathsf{Auger} \to \mathsf{NOT}$ impact ionization
- optical and electrical measurements used
- · extracted lifetimes depend on methods and injection level

-
$$au_{
m SRH}^{
m ll} = au_{
m n}$$
 resp. $au_{
m p}$

-
$$au_{
m SRH}^{
m hl} = au_{
m n} + au_{
m p}$$





SRH Lifetime



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



SRH Lifetime cont'd



• doping induced lifetime reduction

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





SRH Lifetime cont'd



• increased lifetime with increasing temperature

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most common model
 (---) only
 characterized up to 200 K







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

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 $\tau_n \text{: red}, \ \tau_p \text{: blue} \to \text{green} \to \text{purple}$

Auger Recombination



- one investigation dominates coefficients
- reduction with temperature observed

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- Silicon based models (---/ ---/ ---) predict opposite trend





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

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- next up: mobility
- improve presentation and analyses



Conclusion & Outlook



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- next up: mobility
- improve presentation and analyses

Thank you for your attention.







Backup



Silicon Carbide



- wide bandgap material (WBM)
 - one of first investigated semiconductors
 - used in power electronics
 - polytype 4H commonly used
- features high

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- 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 $arepsilon_{
 m r}=arepsilon/arepsilon_0$
- complex relative permittivity

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

- static relative permittivity $\epsilon_{\!s}=\epsilon'(\omega\!\rightarrow\!0)$
- 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

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







- $\epsilon_{\rm s}=\epsilon'(\omega
 ightarrow 0)$ but sometimes $\epsilon_{\!\infty}=\epsilon'(0)$
- 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 ..."





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

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• $\varepsilon_{\mathrm{s}}^{\parallel} > \varepsilon_{\mathrm{s}}^{\perp}$, $\varepsilon_{\infty}^{\parallel} > \varepsilon_{\infty}^{\perp}$

- early investigations on 6H
 - based on data from 1940's

ref.	ϵ_{s}	$arepsilon_{ m s}^{\parallel}$	$\epsilon_{ m s}^{\perp}$	\mathcal{E}_{oo}	\mathcal{E}_{∞}	$arepsilon_{\infty}^{\perp}$	methoda	SiC	doping
[Patr70] ⁵	9.78°	10.03	9.66	6.58°	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°	6.78	6.56	RI	4H	
[Karc96] ¹⁸	10.53°	10.9	10.352	7.02 ^c	7.169	6.946	DFT-LDA	4H	
[Well96] ¹⁹	-	-	-	7.02°	7.17	6.95	DFT-LDA	4H	-

Note: only first entries shown here



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Results cont'd



- [Pern01]⁴⁸ (9.78 / 6.58) - [Pern05]⁴⁹ (9.78 / 6.58) - [Arpa06]⁷⁸ (10/-) [Koiz09]⁵⁰ (10.03 , 9.66 / 6.7 , 6.52) [Scab11a]⁷⁹ (9.78/-) [Naug17]⁸⁰ (10.03, 9.66 / -) - [Arva17]⁸¹ (9.66 / -) [Chou21]⁸² (9.66 / -) - [Yosh18]⁸³ (-, 9.7/-) — [Micc19]⁸⁴ (9.66 / -) - [Trip19]⁸⁵ (9.66 / -) - [Klah20]⁸⁶ (10/-) - [Kova20]⁸⁷ (9.67 / 6.5) — [Ioff23]⁸⁸ (10.03, 9.66 / 6.7, 6.52) - [Acha17]⁸⁹ (8.5884/-) [Bane21]⁹⁰ (8.5884 / -)

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



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





2) Impact Ionization


Theory



• high energy charge carriers create electron-hole pair

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

- impact ionization coefficients [cm⁻¹]
 - β (holes) $> \alpha$ (electrons) [1, 2]

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



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

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

Okuto-Crowell [6]

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

Empirical Models

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



F... electric field [V cm⁻¹]

Physics Based Models

Shockley [7] "lucky electron", low field

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Wolff [8] high field

Thornber [9] arbitrary band structures

$$\alpha, \beta(F) = \frac{eF}{\langle E_i \rangle} \exp\left[-\frac{\langle E_i \rangle}{[(eF\lambda)^2/3E_p] + eF\lambda + E_{k_BT}}\right]$$

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

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

e... elementary charge, E_i... ionization energy

 λ ... mean free path, E_{p} ... optical phonon energy, $E_{k_{\rm B}T}$... thermic phonon energy









 β decreases with increasing temperature

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- increasing α reported
 - compensated by hole temperature dependency
 - $\Delta lpha < \Delta eta$
- few investigations
 - most of them in last decade

TCAD Parameters for 4H-SiC: A Review



Insights



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









3) Incomplete Ionization



Modeling



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

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

• in TCAD tools representation using charge carriers beneficial

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



Lattice sites



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

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

 $E_{\text{Dc}}, E_{\text{Dh}}...$ cubic/hexagonal donor ionization energy $E_{\text{Ac}}, E_{\text{Ah}}...$ 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)

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

Characterization Methods



Hall measurements

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- 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











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









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Additional Analyses



charge carrier cross sections

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· reference chains and value consistency

[Pank14]16 [Zhu08]21 [Neud06]15 200[Bali061165] [Zett02120] [Mart021146 [Neud01]14 [Habe94]166 [Pens93]46 [Kimo19]153 [h] [Nipo18]33 [h] 198 [Kimo14a]164 [h] 197.9 [Janz08]163 [h] [Ioff23]148 [Fan14]150 [Zhan10]160 [Bhat05]86 [Zhao03]161 191 [Wane99]¹⁶² [Pers98]⁵¹ [Greu97]¹⁴⁹ [Bako97]85 [Made91]151 [Yosh18]80 [Megh18]155 190 [Wije]11156 [Nego04]157 [Nego03]158 [Levi01]11 [Gao01]159 150±5+Ex [Hage73]¹³⁸ A1

[Schr06]168 320 ± 20 [Lade00]⁸⁷ [Rakh20]178 [Sull08]179 [Neud06]15 300 [Huh06]180 [Nend01]14 [Gao01]159 [Loph18]58 203 [Dona18]31 [Arva17]154 [Wije11]156 50 [Zhu08]21 285 [Nego03]158 [Zett02]20

280 [Kimo14a]¹⁶⁴

B

single ionization energy values

61	[Yang19] ¹⁸⁶ [Kimo19] ¹⁵³ [h] [Kimo14a] ¹⁶⁴ [h]		[Kimo19]153 [h]		
		60	[Nipo18] ³³ [h]		
60	[Huan22] ²⁹ [Bhat05] ⁵⁶ [h]		[Kimo14a] ¹⁶⁴ [h]		
59	[Levi01] ¹¹ [h] [Iwat01] ¹⁸⁵ [h]		in colline		
55	[Made91] ¹⁵¹ [h]	20	[Son06] [h]		
53	[Gerh11] ¹⁸⁴ [h]				
52.1	[Buon12] ⁵⁹ [h] [Wang99] ¹⁶² [h]	55	[Dona18]31 [h]		
	[Pers99a] ¹⁸³ [h] [Greu97] ¹⁴⁹ [h] [Bako97] ⁸⁵ [h]				
50	(Sec. 10) ¹⁷⁵ (Zha00) ²¹ (b) (Zan02) ²⁰ (b)	54	[Zhu08] ²¹ [h]		
50	[aoxia] [vunos] [u] [vunos] [u]				
$) \pm 5$	[Alba10] ³⁴ [h] [Schr06] ¹⁶⁸ [h]	53	[Zett02] ²⁰ [h]		
$J \perp J$	[Ayal05] ⁸⁸ [h] [Ayal04] ⁶¹ [h] [Lade00] ⁸⁷ [h]	55	[Hand00] ²⁸ [h]		
45	[Wije11] ¹⁵⁶ [Neud06] ¹⁵				
	[Neud01] ¹⁴ [Mick98] ¹⁸² [h]	50 ± 5	[Alba10]34 [h]		
44	[Son06] ¹⁴⁵ [h]				
42	[Zhan10] ¹⁶⁰	45	[Nego04a] ¹⁸⁸		
33	[Pank14] ¹⁶ [h] [Loma74] ¹⁸¹				
Ν		Р			
-					

Note: only first entries shown here





4) Density-of-States Mass



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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

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- conduction band minimum in M-point
- \parallel to c-axis: m^*_{ML}
- \perp to c-axis: $m^*_{
 m M\Gamma}, m^*_{
 m MK}$
- holes
 - valence band maximum in $\Gamma\text{-point}$
 - \parallel to c-axis: $m^*_{\Gamma A}$
 - \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 ($N_{\rm C}$) and valence ($N_{\rm V}$) band

- $M_{\rm C}\ldots$ number of conduction band minima in the first Brillouin zone

$$N_{\rm C} = 2 M_{\rm C} \left(\frac{2\pi m_{\rm de}^* k_B T}{h^2} \right)^{3/2}, \qquad N_{\rm V} = 2 \left(\frac{2\pi m_{\rm dh}^* k_B T}{h^2} \right)^{3/2}$$

• effective masses for electrons (m_{de}^*) and holes (m_{dh}^*)

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

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DOS Mass cont'd



• combine two topmost valence bands

$$m_{\rm dh}^* = \left(m_{\rm hh}^{*3/2} + m_{\rm lh}^{*3/2}\right)^{2/3}$$
.

• ... or even all three

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

• temperature dependency

$$m^{*}(T) = \left(\frac{z_{0} + z_{1}T + z_{2}T^{2} + z_{3}T^{3} + z_{4}T^{4}}{1 + n_{1}T + n_{2}T^{2} + n_{3}T^{3} + n_{4}T^{4}}\right)^{T}$$



[Persson1997] doi:10.1063/1.365578



Polaron Mass



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

$$m_{\rm p} = m \frac{1 - 8 \times 10^{-4} \alpha^2}{1 - \alpha/6 + 3.4 \times 10^{-3} \alpha^2} \approx m \left(1 - \frac{\alpha}{6}\right)^{-1}$$

- Fröhlich constant α
 - term $1/4\pi\epsilon_s$ missing in some publications (differing unit system)

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

 $\epsilon_{\rm s}/\epsilon_{\!\infty}\ldots$ static/high-frequency dielectric constant

 $\omega_{
m LO}\dots$ 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

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- 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

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• heavily based on calculations

- mostly from 1994-2004

.

- two measurements for electrons, none for holes

	electron				hole					
ref.	$m^*_{\rm M\Gamma}$	$m^*_{\rm MK}$	$m^*_{\rm ML}$	band	$m^*_{\Gamma M}$	$m^*_{\Gamma \mathrm{K}}$	$m^*_{\Gamma\Lambda}$	band	methoda	polaron
	$[m_0]$	$[m_0]$	$[m_0]$		$[m_0]$	$[m_0]$	$[m_0]$			
[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





 existing data extended by calculations using masses in principal directions

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- more measurement results found
 - still calculations dominant

	electron				hole					
ref.	$m_{\rm de}^*$	$m^*_{ m de\perp}$	$m^*_{ m de\parallel}$	band	$m_{ m dh}^*$	$m^*_{\mathrm{dh}\perp}$	$m^*_{ m dh\parallel}$	band	methodh	polaron
	[<i>m</i> ₀]	$[m_0]$	$[m_0]$		[<i>m</i> ₀]	$[m_0]$	$[m_0]$			
[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





[Ioff23]⁷⁹ [Scaj13a]³⁷ [Alba10]³⁵ [Resh05]⁹¹

[Pers05]10 [Son04]11 [Lee02]98 [Levi01]81

[Iwat00a]47 [Iwat00]46 [Ivan00]80 [Pers99b]58

[Kino98]50 [Huan98]45 [Pers97]25 [Lamb97]23

[Hemm97]36 [Bako97]18 [Pers96]14 [Nils96]55

[Nils96]55 [Son95]67 [Josh95]101 [Iked80]102

0.35 [Dong04]¹⁷ [Naka97]²⁰ [Lamb95]⁶¹ [Hari95]⁷⁰

[Kim24]95 [Arpa06]96 [Itoh95]97

[Scha94]94 [Pens93]78 [Gotz93]32

[Loma74]73 [Loma73]72

[Rodr21]92 [Kuzn95]93

[Iwat01]48 [Zhao00a]60 [Zhao00]21

0 37 [Pers99a]⁴² [Egil99]³³ [Shah98]⁹⁹ [Pers98a]⁷⁴

[Mick98a]100 [Mick98]75 [Lind98]1

0.36 [Yang19]⁹⁰ [Kuro19]²²

0.32 [Wenz95]56 [Kack94]54

0.34 [Penn01]64

0.33 [Bell00]63

0.20

0.19

 $m_{\rm de}^*$

1.26 [Resh05]⁹¹ [Zhao00]²¹

[Yang19]90 [Alba10]35 [Pere06]103 1.20[Lee02]98 [Shah98]99 [Huan98]45 [Ioff23]⁷⁹ [Neim06]¹¹⁴ [Levi01]⁸¹ [Ivan00]⁸⁰ [Hemm97]³⁶ [Kuzn95]93 [Pens93]78 0.94 [Scai13a]³⁷ [Ishi24]⁴⁴ [Rakh20]¹⁰⁵ [Klah20]¹⁰⁷ 0.91[Kimo14a]108 [Feng04a]111 [Son00]13 [Pear23]104 [Maxi23]82 [Khan23]40 0 82 [Nouk20]¹⁰⁶ [Vasc19]¹¹⁵ [Janz08]¹⁰⁹ [Aval04]15 [Flor03]116 [Lade00]31 0.81 ILamb97123 0.76 [Kuro19]²² 0.50 [Koiz09]71 0.43 [Kack94]⁵⁴ $m_{\rm dh}^*$

Note: only first entries shown here

wide range of values

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- 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



Conductivity Mass



• required for investigations of mobility

$$\mu = rac{e au}{m_c^*}$$

1

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

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





5) Band Gap



Band Gap Energy



band gap $E_{\rm g}$ = exciton band gap $E_{\rm gx}$ + free exciton binding energy $E_{\rm x}$

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







band gap $E_{\rm g}$ = exciton band gap $E_{\rm gx}$ + free exciton binding energy $E_{\rm x}$

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

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



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

$$E_{\rm g}(T) = E_{\rm B} - \alpha_{\rm B} \left(1 + \frac{2}{{\rm e}^{\Theta_{\rm B}/T} - 1} \right)$$

Pässler model

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

- Δ ... phonon dispersion ($\Delta > 1$... Varshni, $\Delta \rightarrow 0$... Bose-Einstein)
- $\Theta_p \dots$ average phonon temperature, $\epsilon \dots$ entropy





• Lindefelt

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$$\begin{split} \Delta E_{\rm g}(N_{\rm D}^+,N_{\rm A}^-) &= -\Delta E_{\rm (n/p)c}(N_{\rm D}^+) + \Delta E_{\rm (n/p)v}(N_{\rm A}^-) \\ \Delta E_{\rm nc}(N_{\rm D}^+) &= A_{\rm nc} \left(\frac{N_{\rm D}^+}{10^{18}}\right)^{1/3} + B_{\rm nc} \left(\frac{N_{\rm D}^+}{10^{18}}\right)^{1/2} < 0 \\ \Delta E_{\rm nv}(N_{\rm D}^+) &= A_{\rm nv} \left(\frac{N_{\rm D}^+}{10^{18}}\right)^{1/4} + B_{\rm nv} \left(\frac{N_{\rm D}^+}{10^{18}}\right)^{1/2} > 0 \\ \Delta E_{\rm pc}(N_{\rm D}^+) &= A_{\rm pc} \left(\frac{N_{\rm A}^-}{10^{18}}\right)^{1/4} + B_{\rm pc} \left(\frac{N_{\rm A}^-}{10^{18}}\right)^{1/2} < 0 \\ \Delta E_{\rm pv}(N_{\rm D}^+) &= A_{\rm pv} \left(\frac{N_{\rm A}^-}{10^{18}}\right)^{1/3} + B_{\rm pv} \left(\frac{N_{\rm A}^-}{10^{18}}\right)^{1/2} + C_{\rm pv} \left(\frac{N_{\rm A}^-}{N_{\rm A0}}\right)^{1/4} > 0 \end{split}$$



Doping Dependency cont'd



Slotboom

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

Schubert

- not able to reproduce plots found in literature

$$\Delta E_{
m g} = rac{e^3\sqrt{n}}{4\piarepsilon^{3/2}\sqrt{k_{
m B}T}}$$
 $\Delta E_{
m g} = rac{e^3\sqrt{m_{
m de}^*(3n)^{1/3}}}{4\pi^{5/3}arepsilon^{3/2}\hbar}$

(Debye, non-degenerate)

(Thomas-Fermi, degenerate)





• optical measurements

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- 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
 - $E_{gx} = 3.265(2) \text{ eV}$
- · latest calculations predict clearly lower values
 - $E_g = 3.15(3) \, \text{eV}$

		band gap		ļ	temperature de	p.		
ref.	E_{g}	$E_{\rm gx}$	$E_{\rm x}$	Tg	α	β	interval	method ⁸⁰
	[eV]	[eV]	[meV]	[K]	$[eVK^{-1}]$	[K]	[K]	
[Choy57] ^{59 81}	-	-	-	-	$3.3 imes 10^{-4}$	-	-	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

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too few measurements to verify







Temperature Dependency

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





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Band Gap Values



- overwhelming amount of values in literature
 - very few temperature scaling parameters
 - $E_{g}(T_{g})$ 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 $E_{
 m gx}
 ightarrow E_{
 m g}$
 - coincidentally measurement of $E_{\rm g}(300) \approx 3.26\,{\rm eV}$
- future research
 - room temperature measurements for verification
 - temperature dependency of $E_{\rm X}$

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6) Charge Carrier Recombination

Characterization Methods



optical measurements

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- (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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