TCAD Parameters for 4H-SiC: A Review

Band Gap

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Literature Review

- goals
  - lower entrance barrier for newcomers
  - critical evaluation of status quo
- methods
  - present published models/parameters
  - check consistency with references
  - identify key publications and values
  - distinguish hexagonal/cubic lattice sites and direction $\perp$ / $\parallel$ to c-axis
- data analysis finished
  - comments/suggestions still possible
- chapters made available at https://jburin.web.cern.ch
- now also on arXiv:2410.06798

Topics

✓ relative permittivity (24/10/07)
  - $\varepsilon^{\parallel}, \varepsilon^{\perp}, \varepsilon_{\infty}^{\parallel}, \varepsilon_{\infty}^{\perp}$

✓ impact ionization (24/10/07)
  - empirical and physics based models

✓ incomplete ionization (24/10/21)
  - doping and temp. dependency

✓ density-of-states mass (24/10/21)
  - calculations and measurements

- band gap
  - (exciton) bandgap energy

- mobility
  - low and high field, saturation velocity
- charge carrier recombination
  - SRH, bimolecular and Auger

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

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

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

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

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

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

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

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Doping Dependency cont'd

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- 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

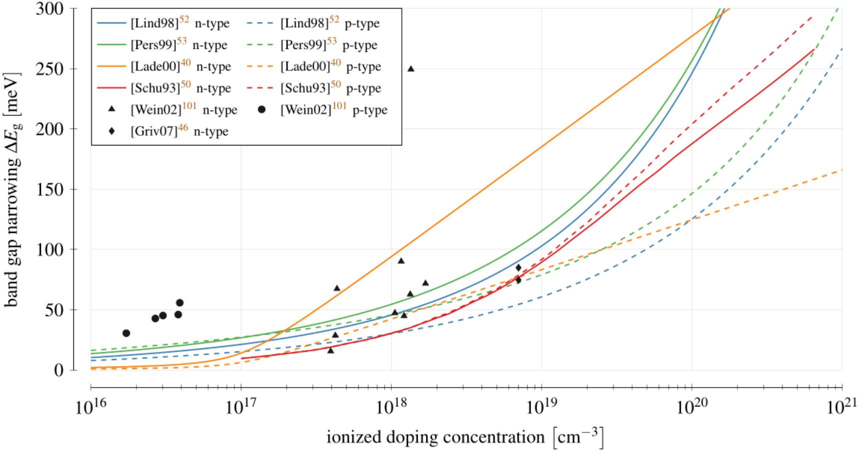
- measurements mainly of E_{gx} at low temperatures
  - $E_{gx} = (3.265 \pm 0.002)$ eV
- latest calculations predict clearly lower values
  - $E_g = (3.15 \pm 0.03)$ eV

ref.	band gap E_g [eV]	E_{gx} [eV]	E_x [meV]	temperature dep. 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

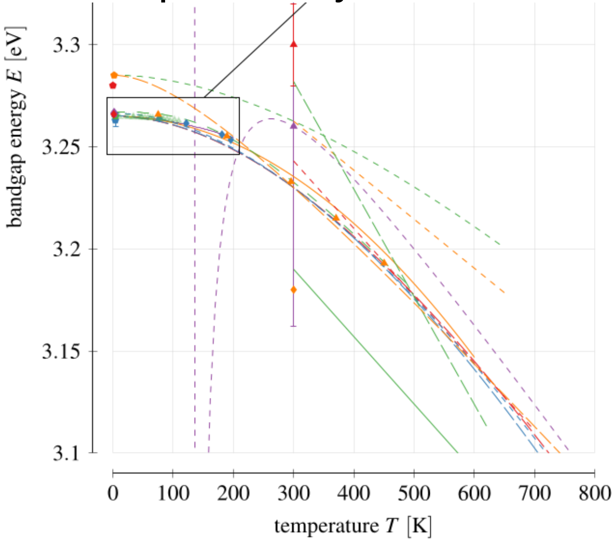
Doping Dependency

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



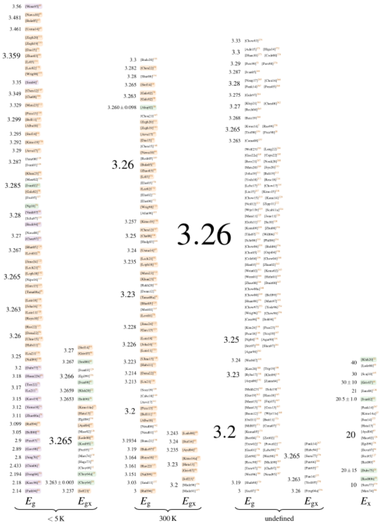
Temperature Dependency

- 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
  - $E_g(T_g)$ 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 $E_{gx} \to E_g$
  - coincidentally measurement of $E_g(300) \approx 3.26$ eV
- future research
  - room temperature measurements for verification
  - temperature dependency of E_x



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Conclusion & Outlook

- band gap
  - excitonic, temperature and doping dependency
  - currently used values go back to measurements in 1964
  - coincidentally seem fitting
  - future research required for confirmation
- combined work available on arXiv:2410.06798
- outlook
  - next up: charge carrier recombination

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Thank you for your attention.

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