TCAD Parameters for 4H-SiC: A Review

Introduction & Relative Permittivity & Impact Ionization

Jürgen Burin, Philipp Gaggl, Simon Waid, Andreas Gsponer and Thomas Bergauer

juergen.burin@oeaw.ac.at, https://jburin.web.cern.ch

Institute of High Energy Physics (HEPHY), Austrian Academy of Sciences

5th General WG4 Meeting, October 7th 2024

Motivation

- TCAD simulations
  - which models?
  - what parameter values?
- challenges for 4H-SiC
  - overwhelming amount of data
  - high anisotropy resp. to c-axis

Symbol	Keyword	Type	Unit
μ_{300}^{min}	uLImin300	Quantity	$cm^2V^{-1}s^{-1}$
γ_1	uLIexpTabove	Real	
γ_2	uLIexpTbelow	Real	
T_{switch}	Tswitch	Quantity	K
C_{300}^{ref}	Cref300	Quantity	cm^{-3}
γ_3	CrefexpT	Real	
α_{300}	alpha300	Real	
γ_4	alphaExpT	keywordReal	

Table 6.25.: Caughey-Thomas mobility model keywords

ÖAW AUSTRIAN ACADEMY OF SCIENCES

Literature Review

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS

- 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

Topics

- relative permittivity
  - $\varepsilon^{\parallel}, \varepsilon^{\perp}, \varepsilon_{\infty}^{\parallel}, \varepsilon_{\infty}^{\perp}$
- impact ionization
  - empirical and physics based models
- (temperature dependent) bandgap
  - (exciton) bandgap energy
- mobility
  - low and high field, saturation velocity
- effective electron/hole masses
  - calculations and measurements

- incomplete ionization
  - doping and temp. dependency
- generation/recombination
  - SRH, bimolecular and Auger

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

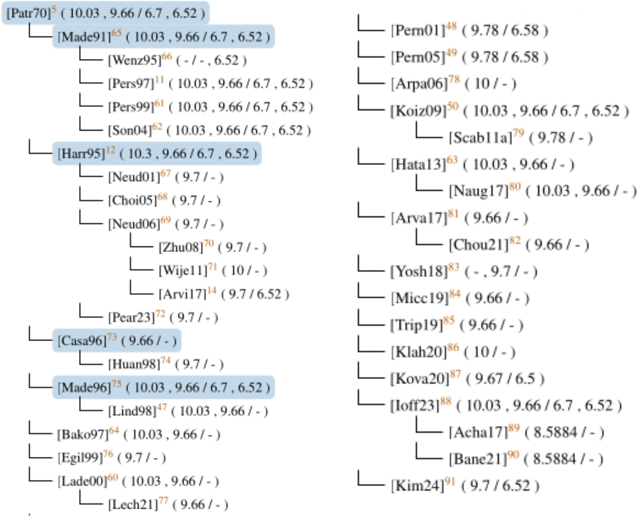
- many fundamental investigations identified
  - measurements and calculations
  - still active field of research
- $\varepsilon_\mathrm{s}^{\|} > \varepsilon_\mathrm{s}^{\perp}$, $\varepsilon_\infty^{\|} > \varepsilon_\infty^{\perp}$
- early investigations on 6H
  - based on data from 1940's

ref.	ε_s	$\varepsilon_\mathrm{s}^{\|}$	$\varepsilon_\mathrm{s}^{\perp}$	ε_∞	$\varepsilon_\infty^{\|}$	$\varepsilon_\infty^{\perp}$	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

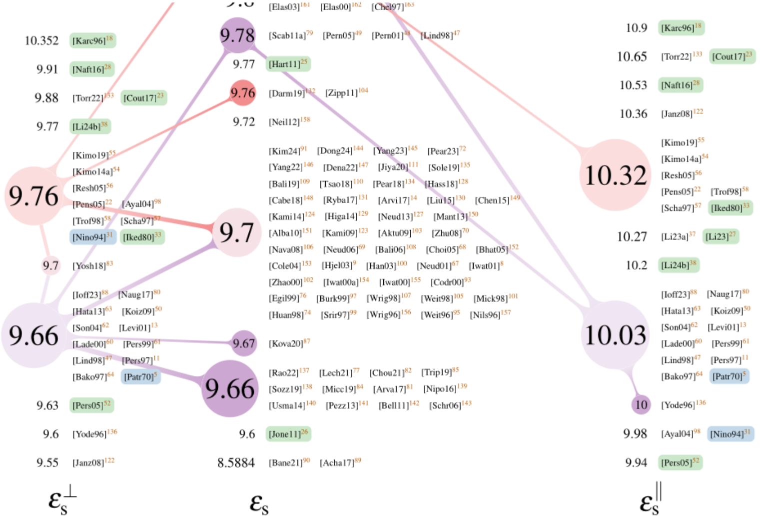
Results cont'd

- 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]

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

ÖAW AUSTRIAN ACADEMY OF SCIENCES

Empirical Models

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS

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
$a \rightarrow a\gamma$, $b \rightarrow b\gamma$

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

$F\ldots$ 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

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

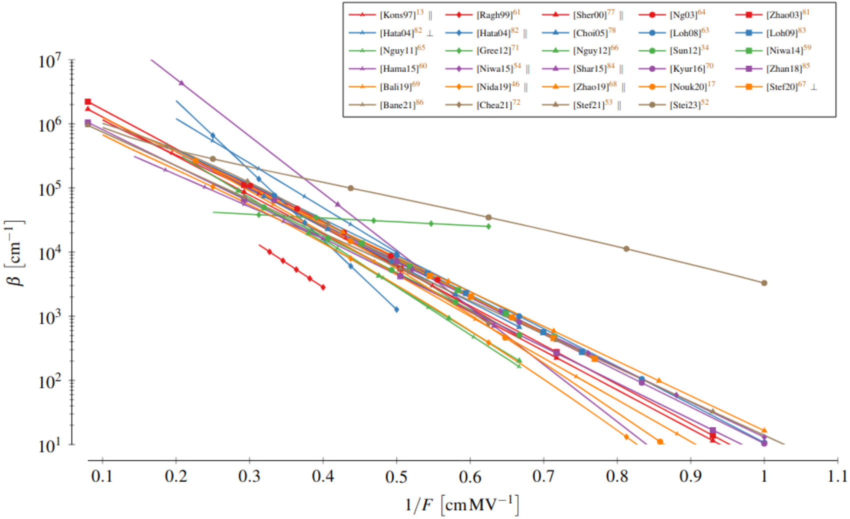
Thornber [9]
arbitrary band structures

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

$e \ldots$ elementary charge, $E_\mathrm{i} \ldots$ ionization energy
$\lambda \ldots$ mean free path, $E_\mathrm{p} \ldots$ optical phonon energy, $E_{k_\mathrm{B}T} \ldots$ thermic phonon energy

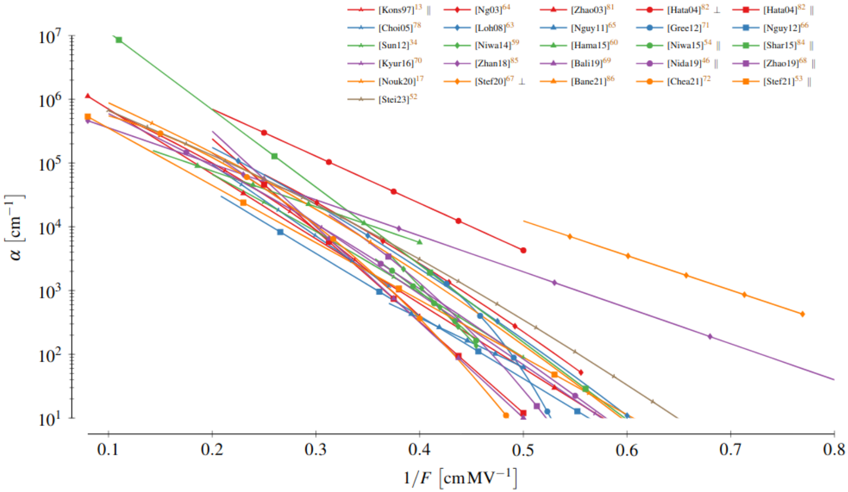
Results Holes

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



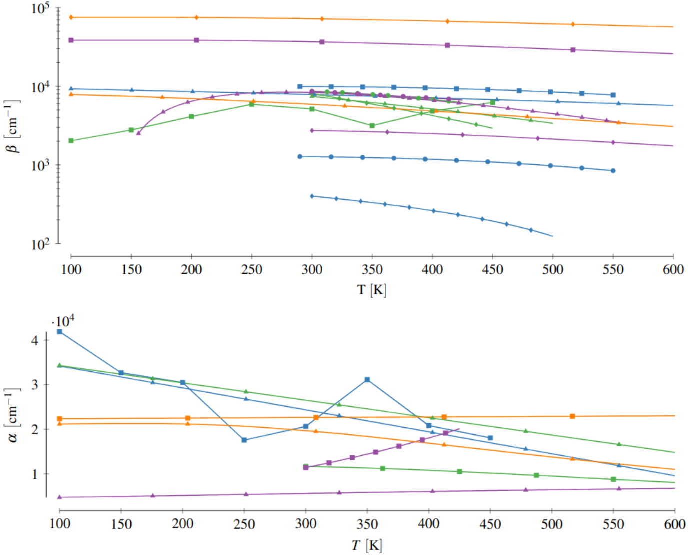
Results Electrons

- 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



ÖAW AUSTRIAN ACADEMY OF SCIENCES

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS

Insights

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

Okuto Crowell $(\underbrace{a_\perp, a_\parallel / b_\perp, b_\parallel / m}_{\text{electron}} \mid \underbrace{a_\perp, a_\parallel / b_\perp, b_\parallel / m}_{\text{hole}})$

Kyuregyan and Yurkov

- [Kyur89][93] (457 / 52.4 / 1 | 5.13 / 15.7 / 1)
  - [Ioff23][99] (457 / 52.4 / 1 | 5.13 / 15.7 / 1)

Trew, Yan, and Mock

- [Trew91][94] (0.046 / 12 / 1 | 4.65 / 12 / 1)
  - [Wrig96][95] (0.046 / 12 / 1 | 4.65 / 12 / 1)
    - [Wrig98][96] (0.046 / 12 / 1 | 4.65 / 12 / 1)
      - [Bhat05][97] (0.046 / 12 / 1 | 4.65 / 12 / 1)

Bakowski, Gustafsson, and Lindefelt

- [Bako97][2] (1.41 , 4.95 / 2.58 / 1 | 21.6 , 21.6 / 19 / 1)
  - [Lade00][56] (3.44 / 2.58 / 1 | 32.4 / 19 / 1)
    - [Ayal04][57] (3.44 / 25.8 / 1 | 3.5 / 17 / 1)
      - [Trip19][100] (3.44 / 25.8 / 1 | 3.5 / 17 / 1)
    - [Schr06][92] (3.44 / 2.58 / 1 | 32.4 / 19 / 1)

Hatakeyama *et al.*

- [Hata04][82] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
  - [Hata04a][109] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
  - [Hata05][110] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
    - [Ivan09][111] (- / - / - | - / 25 / -)
    - [Loph18][112] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
    - [Jin24][45] (21 , 176 / 17 , 33 / 1 | - / - / -)
  - [Hata09][44] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
    - [Hata13][113] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
      - [Naug17][114] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
    - [Sole19][115] (210 , 176 / 17 , 33.3 / 1 | 296 , 341 / 16 , 25 / 1)
  - [Buon12][3] (210 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
  - [Chen15][116] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
  - [Megh15][117] (21 , 176 / 17 , 33 / 1 | 29.6 , 241 / 16 , 25 / 1)
  - [Wang22][118] (21 , 176 / 17 , 33 / 1 | 29.6 , 341 / 16 , 25 / 1)
  - [Yang23][119] (- / - / - | - / - / -)

Loh *et al.*

- [Loh08][63] (2.78 / 10.5 / 1.37 | 3.51 / 10.3 / 1.09)

Note: only first entries shown here

ÖAW AUSTRIAN ACADEMY OF SCIENCES

Conclusion & Outlook

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS

- TCAD parameter review of 4H-SiC
  - overview and critical evaluation
  - literature often confusing
- relative permittivity
  - old and 6H values commonly used
  - wide range of values found in literature
- impact ionization
  - holes bigger impact than electrons
- outlook
  - chapters made available at https://jburin.web.cern.ch and here

Conclusion & Outlook

- TCAD parameter review of 4H-SiC
  - overview and critical evaluation
  - literature often confusing
- relative permittivity
  - old and 6H values commonly used
  - wide range of values found in literature
- impact ionization
  - holes bigger impact than electrons
- outlook
  - chapters made available at https://jburin.web.cern.ch and here

Thank you for your attention.

References

[1] Sadao Adachi. *Properties of Group-IV, III-V and II-VI Semiconductors*. Chichester, England: John Wiley, 2005. ISBN: 978-0-470-09032-9.

[2] T.P. Chow et al. “SiC and GaN Bipolar Power Devices”. In: *Solid-State Electronics* 44.2 (Feb. 2000). ISSN: 00381101. DOI: 10.1016/S0038-1101(99)00235-X.

[3] A. G. Chynoweth. “Ionization Rates for Electrons and Holes in Silicon”. In: *Physical Review* 109.5 (Mar. 1, 1958). ISSN: 0031-899X. DOI: 10.1103/PhysRev.109.1537.

[4] A. G. Chynoweth. “Uniform Silicon *P-n* Junctions. II. Ionization Rates for Electrons”. In: *Journal of Applied Physics* 31.7 (July 1, 1960). ISSN: 0021-8979, 1089-7550. DOI: 10.1063/1.1735795.

[5] R. Van Overstraeten and H. De Man. “Measurement of the Ionization Rates in Diffused Silicon P-n Junctions”. In: *Solid-State Electronics* 13.5 (May 1970). ISSN: 00381101. DOI: 10.1016/0038-1101(70)90139-5.

[6] Y. Okuto and C.R. Crowell. “Threshold Energy Effect on Avalanche Breakdown Voltage in Semiconductor Junctions”. In: *Solid-State Electronics* 18.2 (Feb. 1975). ISSN: 00381101. DOI: 10.1016/0038-1101(75)90099-4.

[7] William Shockley. “Problems Related to P-n Junctions in Silicon”. In: *Solid-State Electronics* 2.1 (Jan. 1961). ISSN: 00381101. DOI: 10.1016/0038-1101(61)90054-5.

[8] P. A. Wolff. “Theory of Electron Multiplication in Silicon and Germanium”. In: *Physical Review* 95.6 (Sept. 15, 1954). ISSN: 0031-899X. DOI: 10.1103/PhysRev.95.1415.

[9] K. K. Thornber. “Applications of Scaling to Problems in High-Field Electronic Transport”. In: *Journal of Applied Physics* 52.1 (Jan. 1, 1981). ISSN: 0021-8979, 1089-7550. DOI: 10.1063/1.328490.

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