



TCAD Parameters for 4H-SiC: A Review Band Gap

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

7th General WG4 Meeting, November 11th 2024

Literature Review



• goals

ADEMY OF

- 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





CADEMY OF





- ✓ relative permittivity (24/10/07)
 - $\varepsilon^{\parallel}, \varepsilon^{\perp}, \varepsilon^{\parallel}_{\infty}, \varepsilon^{\perp}_{\infty}$
- ✓ 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 $E_{\rm g}$ = 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 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

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



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, $\mathcal{E} \dots$ entropy





• Lindefelt

۸۱۸

AUSTRIAN ACADEMY OF SCIENCES

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



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

AUSTRIAN

- 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







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

		band gap			temperature de			
ref.	$E_{\rm g}$	E_{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

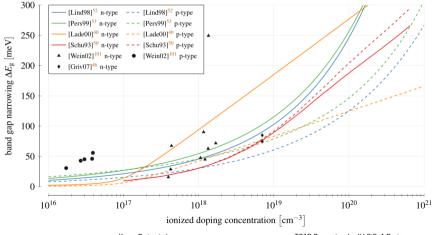


• increasing narrowing with doping concentration

AUSTRIAN

SCIENCES

too few measurements to verify



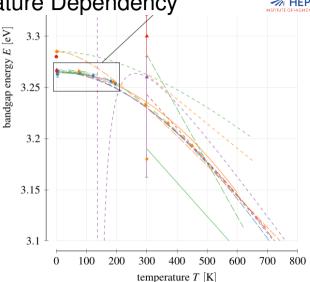
Jürgen Burin et al.





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





CADEMY OF

CIENCES

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 $E_{\rm X}$

3.481	NAUE"													
3.461	(Ereal C)*													
	CRUMPS"							1.15	Ebox3					
	Dealer -								IA RUTO	Date:				
3.359	Peed a			3.3	INA.117**				Parts (
	(L+42)**			3.282	(Cheal.2)**				Posts ¹ I	Parallel				
	(Waght) **				(8x91)**				Pring 171					
	(Decipi *				Distant"				Poloti	Postfill				
3.349	(Durin) ^{**}			3.263	104.007				Kinger Q					
3.329	(Mail)*			3.260 ± 0.096				3.27	Britel,	Chiefe,				
3.299	0.811				Kholi I." Kupi I.			3.268	Bottle					
	Date 11				(Kapite)			3.265	Krett/	Barth				
	(Keed C				East V			3.263	Case 10					
	Chesty				(Card I) *				1918(1)**	Log(1) ⁱⁿ				
3.367	(heating) ^(a)			2.24	BURG				Field,"					
	(hadd)*			3.26	DAGY .				MACON PALES	Rents				
	(Martil) ¹⁰				8.001				Pink #	Berthfill				
3.285	(head)				Red T				E-bitting	Chair.				
	(RAAD)*				First of T				EAST 1	Kan CT				
	(Note)				Elsest.				Plot 2/**	Sec. 1				
3.28	(PARTY T				(Majer)**					Plot in the				
3.28	18.8417			3.247	Non-Pri				Mexil [®]	(how 1)				
	(Buddy"				Chod 3	^	γ	r -	Name of Street o	(Fedd)"				
3.27	(Reide)*			3.25	Christian .	- 1	.26	۱.	PLANT .	(h)(k)				
	(Multiple)				beful.	-	(·						
3.267	(Long)				Planet-Q				Ebold Conce	physics) ¹⁰⁰				
	(hash)			3.235	Lok31 Lyhte									
	(LA.B.) 8 ¹¹ (LAB) 81 ⁻¹				(And L'				(Real()))	Sead (P				
3.265	West W				(Khai) 1 ²⁴				(Real (** (Real (**	Panet -				
	(Res 11)"				PANY"									
	(8.410.8)**			3.23	(Textifie)*				Floring Page 10	(8.184)				
3.263	(halo)				(Rect)				there's	(Kahne)**				
3.263	CLARE DI P				Rand S				184/87	Shadd?"				
	(Repurp) ?			3.228	(Reality 7				Easter"					
	(Band Of			3.228	Khard Film				Rabi*	Proch				
3.26	(Desiff"			3 834	EADY .		1	3.25	Pup 4"* 1	Acres -				
	BALL T	3.27	Charles .	3.226	ELAL S				JAANEY"	(Denil 1)**				
3.25	(BUBR)*	1.047	Charles	3.223	"Jints				(Rune)				40	POADE
3.2	(Berry ?)	3.867	Dark 1		BALLY.				Bar21"	12410				Radow P
3.18	(Really)	3.266	(Fg.244)**		Ewold."			3.23	BANDY"	80.017*				Phage 2
3.17	(7+11)		(hutter)	3.213	RACE?				NABLY*				30 ± 10	
	(LAZI)		(65431		Kauter -									Fault (**
	(Kaster) (Famile)	3.2633	(Kendal)		Pour P				Max 11"				20.5 ± 1.0	Public
	(Darde)			3.2	(BALLY T				Beatly!*	(Not be the				Plant 4.0"
	(Bullet)		12,000		(Advertight)				ENE UP	Bell				Post I
	(5.897)		(Nov421*		(PALAR) **	3.243 (5.44)	- 3.	2	Bendry				20	Paul V
	(Feed 1)	3.265	Laber?	3.1934	(freedorf **	3.24 (845)	, J.	4	Bonk/*	(Long)		Partie	20	Photo: *
	(Karnet	0.000	(Post of Carlot		maint	3.235 (Aul			Kaster*	LAW		Parts -		Faral C
2.8	(heg b)		(Nec14)*	3.164	Real V	(K.m.	ind"		Date?"	No. of Concession, Name	3.265	(ken T)		F= #11"
2.433	(Date)		(Rev1)*	3.161	Bard?"	3.23 (84)	R[¹]		Russi'	P8.8.91		(hank)**	22 ± 15	Brooki,
	(heptic)		(During"		(MANY -	2044			(faith)		3.263	Tent"	29 ± 15	BARD?
		3.263 ± 0.003			(Ned 1)	3.2 min	10.0		(Date)*			(mare)	10	(kaul 1)
2.14	(Publik)*	3.237		3	pane"	(Made	10 P		period.		3.25	Proping **		panta;**
	E_{2}		Egx		E_{g}	E_{g}	x.		E_g			Egx		E_x
<u> </u>		~					_	_		~				
		< 5 K				100 K				undefi	ned			



Conclusion & Outlook



• band gap

AUSTRIAN

CIENCES

- 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



Conclusion & Outlook



• band gap

CADEMY OF

CIENCES

- 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

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

AUSTRIAN

SCIENCES

- charge carrier mobilities
- breakdown field
- thermal conductance
- utilization @ HEPHY
 - low noise particle detector
 - medical and HEP applications

