Structure and Polytypes of Silicon Carbide

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MATRL 286G

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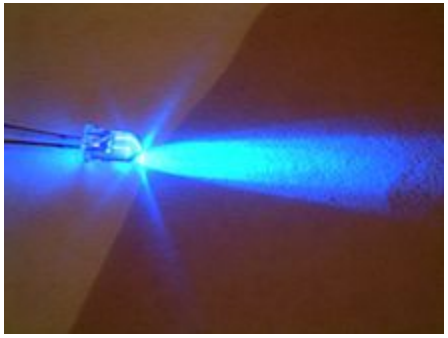
Wide range of applications of SiC

Cutting disks

Body armor

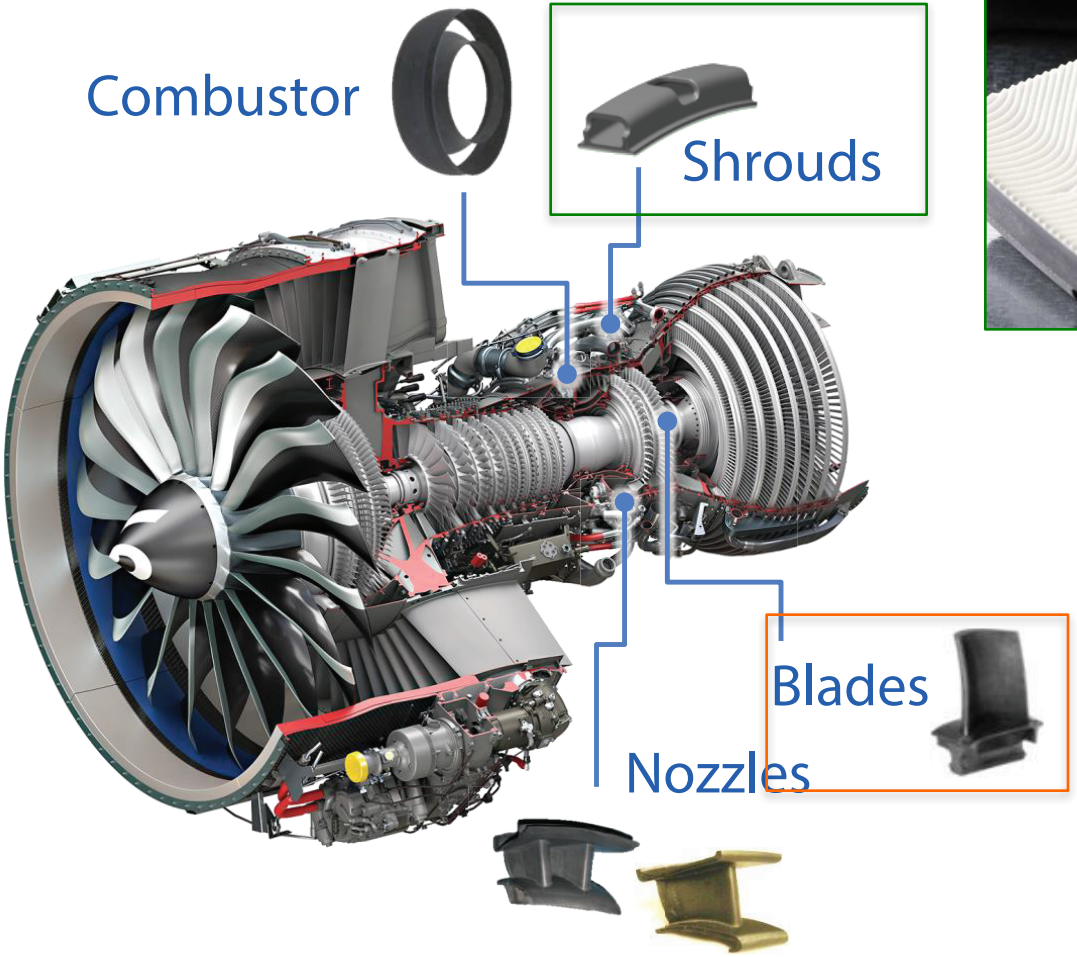
Disc brakes



LEDs

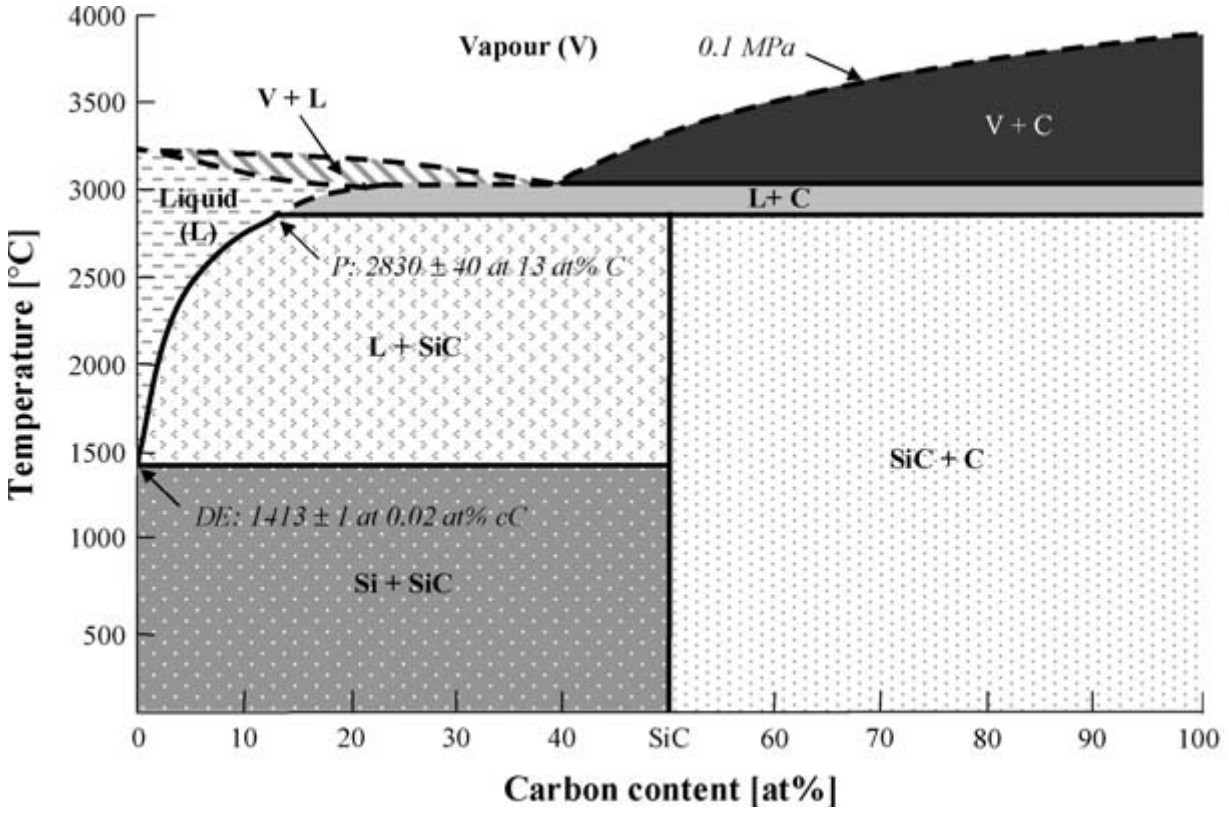
https://en.wikipedia.org/wiki/Silicon_carbide

SiC-SiC Ceramic matrix composites (CMCs) in jet engines



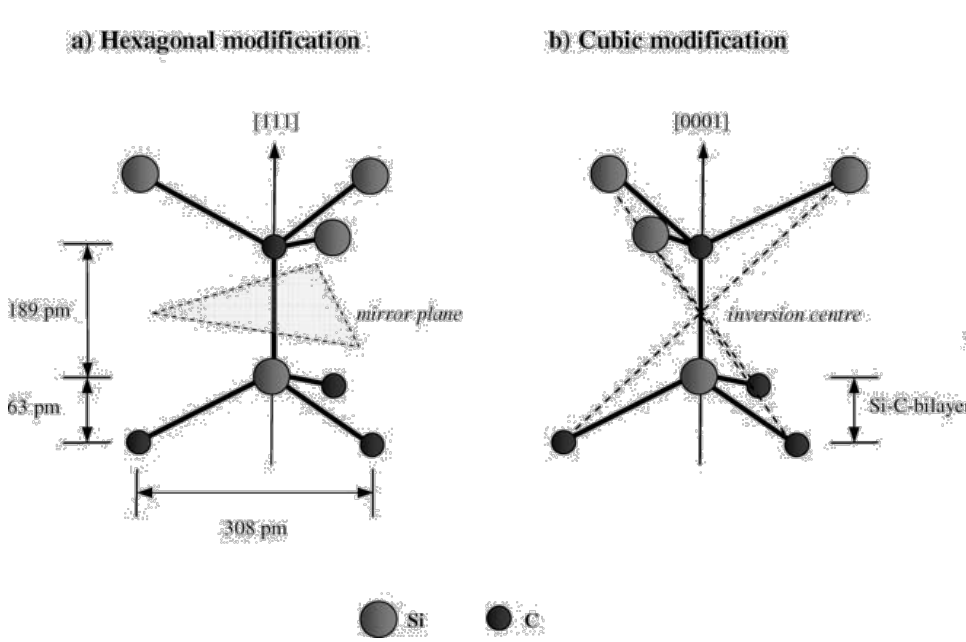
GE Aviation

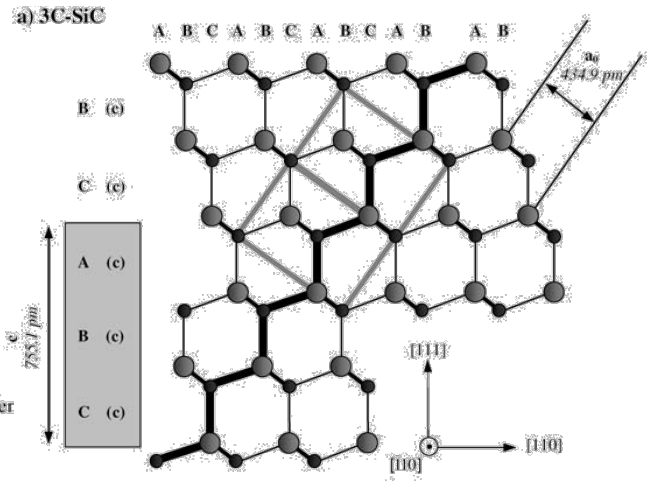
Phase diagram of Si and C

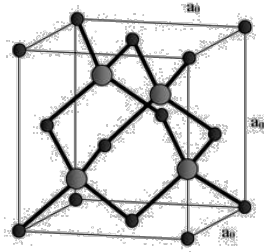


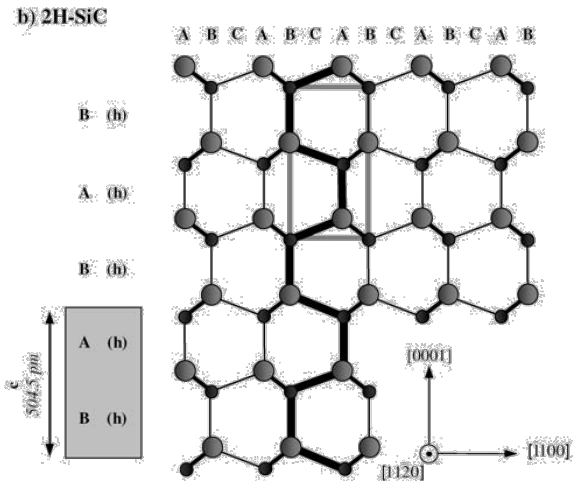
V. Presser and K. G. Nickel (2008), Critical Reviews in Solid State and Materials Sciences, 33:1, 1-99

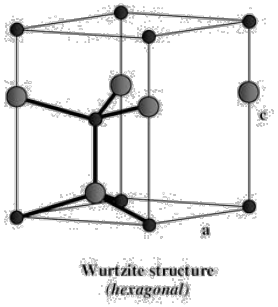
Structure of SiC







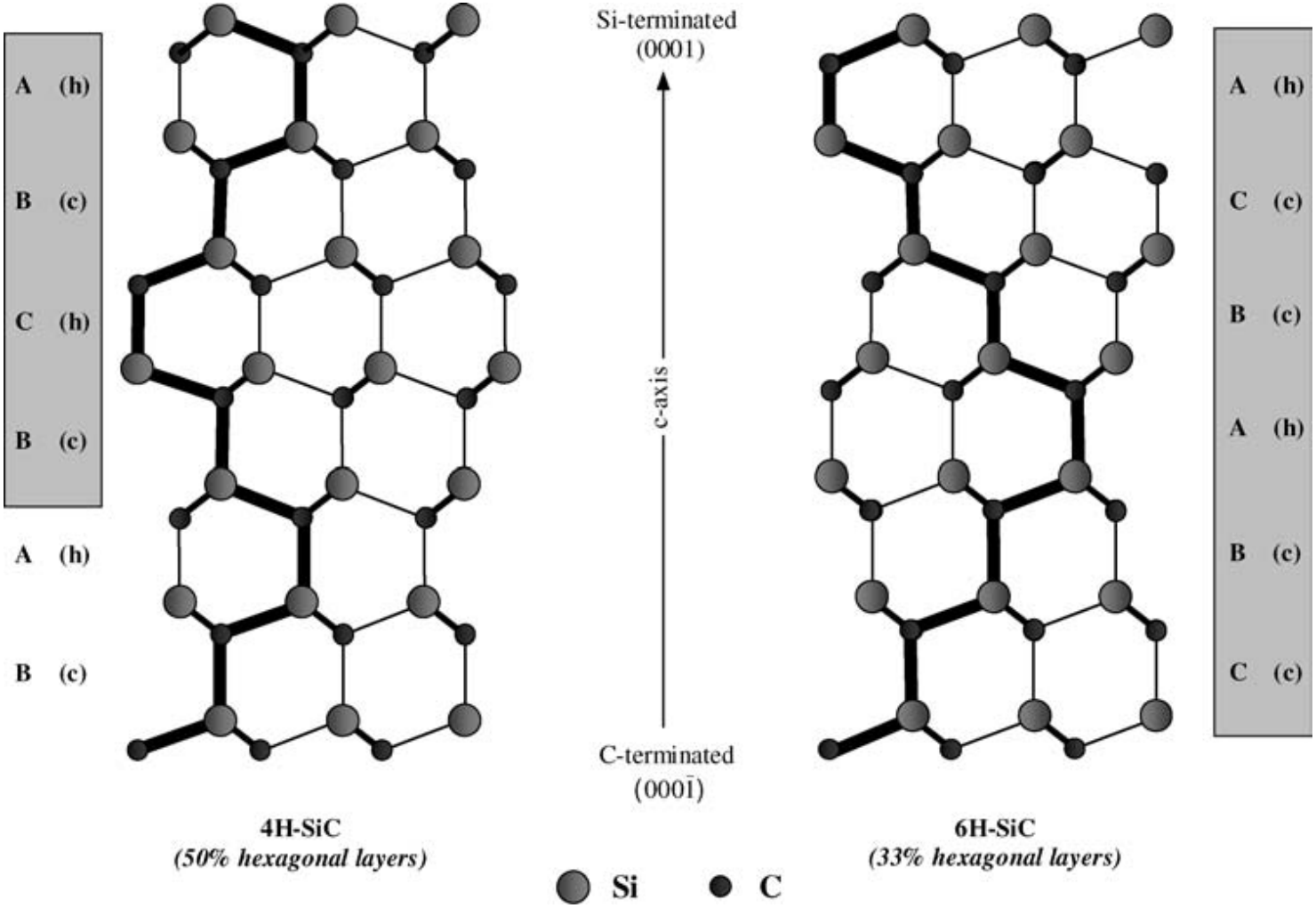




- Si_4C or C_4Si tetrahedra are basic building blocks of SiC
- Stacking of the Si-C bilayers result in various possible polytypes
- Polytypes: identical in two dimensions and differ in the third

V. Presser and K. G. Nickel (2008), Critical Reviews in Solid State and Materials Sciences, 33:1, 1-99

Mixed cubic and hexagonal stackings



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Polytype nomenclature

R	Stacking order	J	ZH	Hex.	SG	Z
3C	abc	(k)	(∞)	0.00	F $\bar{4}$3m	2
6H	abcacb	$(hkk)_2$	(33)	0.33	P 6_3mc	12
15R	abacbcacbabcbac	$(hkhkk)_3$	$(32)_3$	0.40	R 3m	10
4H	abcb	$(hk)_2$	(22)	0.50	P 6_3mc	8
2H	abab	$(h)_2$	(11)	1.00	P 6_3mc	4

R: Ramsdell notation
nX where n = total number of layers and X = *H* , *R* or *C* to indicate the lattice type (hexagonal, rhombohedral, or cubic)

J: Jagodzinski notation
Cubic (k) and hexagonal (h) tetrahedra stacking order

ZH: Zhdanov Hex notation
Zigzag-pattern (forward and backward) along the stacking-order

Hexagonality: ratio of k to n

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Some of the known polytypes (total number: ~250)

Polytype	Space group	Z	Pearson symbol	SgNo	a (Å)	c (Å)	Bandgap (eV)	Hexagonality (%)
3C	T^2_d-F43m	2	cF8	216	4.3596	4.3596	2.3	0
2H	C^4_{6v}-P6_3mc	4	hP4	186	3.0730	5.0480	3.3	100
4H	C^4_{6v}-P6_3mc	8	hP8	186	3.0730	10.053	3.3	50
6H	C^4_{6v}-P6_3mc	12	hP12	186	3.0730	15.11	3.0	33.3
8H	C^4_{6v}-P6_3mc	16	hP16	186	3.0730	20.147	2.86	25
10H	P3m1	10	hP20	156	3.0730	25.184	2.8	20
19H	P3m1	19	hP38	156	3.0730	47.8495		
21H	P3m1	21	hP42	156	3.0730	52.87		
27H	P3m1	27	hP54	156	3.0730	67.996		
36H	P3m1	36	hP72	156	3.0730	90.65		
9R	not found	9	hR18	160	3.073			66.6
15R	C^5_{3v}-R3m	15	hR30	160	3.073	37.7	3.0	40
21R	C^5_{3v}-R3m	21	hR42	160	3.073	52.89	2.85	28.5
24R	C^5_{3v}-R3m	24	hR48	160	3.073	60.49	2.73	25
27R	C^5_{3v}-R3m	27	hR54	160	3.073	67.996	2.73	44
33R	C^5_{3v}-R3m	33	hR66	160	3.073	83.11		36.3
45R	C^5_{3v}-R3m	45	hR90	160	3.073	113.33		40
51R	C^5_{3v}-R3m	51	hR102	160	3.073	128.437		35.3
57R	C^5_{3v}-R3m	57	hR114	160	3.073	143.526		
66R	C^5_{3v}-R3m	66	hR132	160	3.073	166.188		36.4
75R	C^5_{3v}-R3m	75	hR150	160	3.073	188.88		
84R	C^5_{3v}-R3m	84	hR168	160	3.073	211.544		
87R	C^5_{3v}-R3m	87	hR174	160	3.073	219.1		
93R	C^5_{3v}-R3m	93	hR186	160	3.073	234.17		
105R	C^5_{3v}-R3m	105	hR210	160	3.073	264.39		
111R	C^5_{3v}-R3m	111	hR222	160	3.073	279.5		
120R	C^5_{3v}-R3m	120	hR240	160	3.073	302.4		
141R	C^5_{3v}-R3m	141	hR282	160	3.073	355.049		
189R	C^5_{3v}-R3m	189	hR378	160	3.073	476.28		
393R	C^5_{3v}-R3m	393	hR786	160	3.073	987.60		

https://en.wikipedia.org/wiki/Polymorphs_of_silicon_carbide

Polytypism occurs because the difference in energy between the cubic and hexagonal stacking is small

Physicochemical and mechanical properties are almost identical between polytypes, but large variation electrical structure.

Unanswered fundamental problems concerning polytypes: Many stackings should occur, so why are there not infinitely many and why are they not disordered?

Cubic and hexagonal band structure

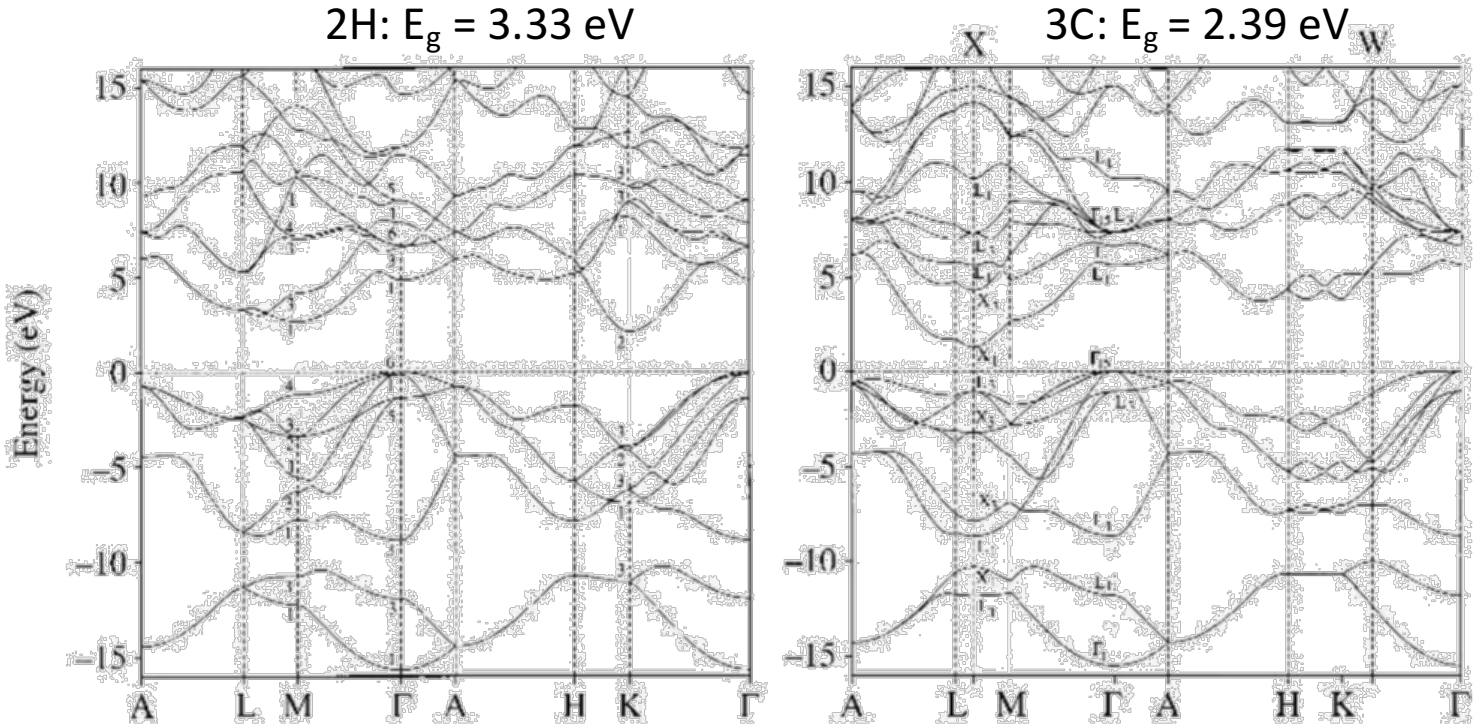
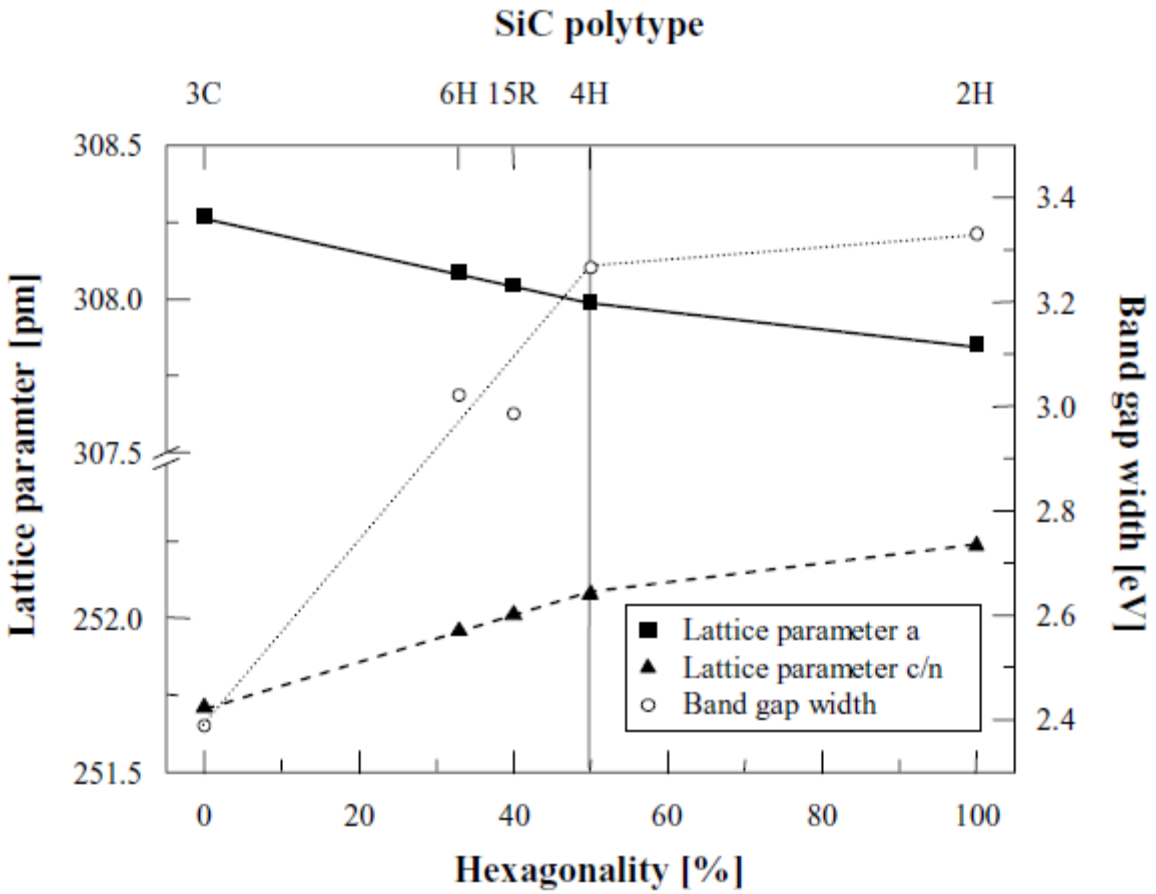


Fig. 5. Band structures of 2H (left) and 3C (right) SiC, both shown in the 2H Brillouin zone. In the right panel, the locations of some cubic high-symmetry points are indicated by additional vertical dashed lines, labeled at the top. The labeling of states is that for the cubic symmetry in the right panel and for hexagonal symmetry in the left

~1 eV difference in E_g
Other materials with polytypes often differ by < 0.1 eV (e.g. ZnS)

W. R. L. Lambrechts, S. Limpijumnong, S. N. Rashkeev, and B. Segall, *Phys. Stat. Sol. (b)* **202**(1), 5, (1997).

Band gap and lattice parameter dependence on hexagonality



- Brillouion zone folding is the origin of the linear dependence of the gap on hexagonality
- Hexagonality contorts unit cell, decreasing *a* and increasing *c/n*

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Conclusions

- Structure of SiC built on stacking of Si_4C and C_4Si tetrahedra
- Many physicochemical and mechanical properties depend on average values, so not affected by structural differences
- Electrical structure depends on geometry (1 eV difference in band gap from cubic to hexagonal)
- Band gap range and high temperature stability allow SiC to be potentially used as a semiconductor enabling operation of devices at high-temperatures, high-power, and high-frequencies
- Remaining questions: why are there not infinitely many polytypes and why are they not disordered?