Polymorphs of silicon carbide

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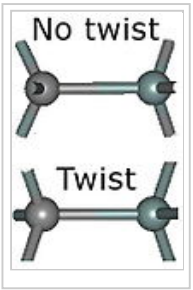
Many compound materials exhibit polymorphism, that is they can exist in different structures called polymorphs. Silicon carbide (SiC) is unique in this regard as more than 250 **polymorphs of silicon carbide** had been identified by 2006,[1] with some of them having a lattice constant as long as 301.5 nm, about one thousand times the usual SiC lattice spacings.[2]

The polymorphs of SiC include various amorphous phases observed in thin films and fibers,[3] as well as a large family of similar crystalline structures called **polytypes**. They are variations of the same chemical compound that are identical in two dimensions and differ in the third. Thus, they can be viewed as layers stacked in a certain sequence. The atoms of those layers can be arranged in three configurations, A, B or C, to achieve closest packing. The stacking sequence of those configurations defines the crystal structure, where the unit cell is the shortest periodically repeated sequence of the stacking sequence. This description is not unique to SiC, but also applies to other binary tetrahedral materials, such as zinc oxide and cadmium sulfide.

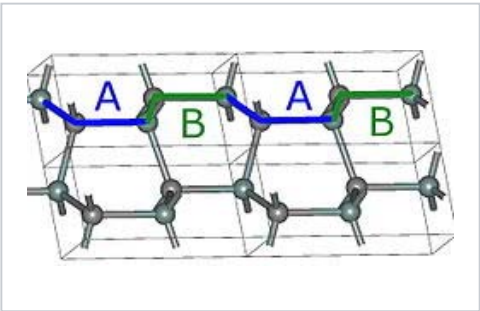
Contents

Categorizing the polytypes

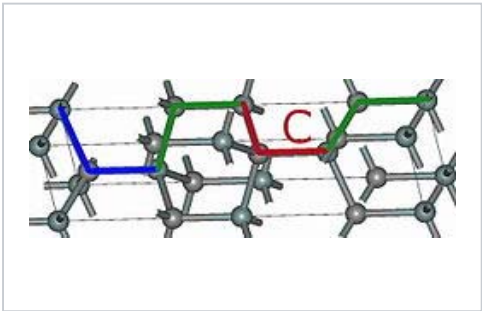
A shorthand has been developed to catalogue the vast number of possible polytype crystal structures: Let us define three SiC bilayer structures (that is 3 atoms with two bonds in between in the pictures below) and label them as A, B and C. Elements A and B do not change the orientation of the bilayer (except for possible rotation by 120° , which does not change the lattice and is ignored hereafter); the only difference between A and B is shift of the lattice. Element C, however, twists the lattice by 60° .



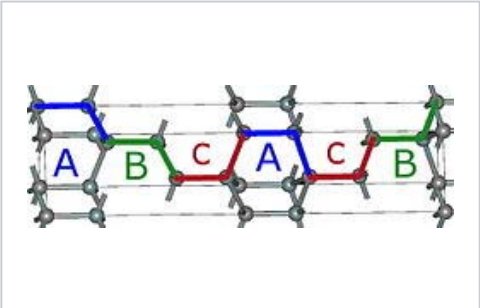
Structure of major SiC polytypes.



2H-SiC



4H-SiC



6H-SiC

Using those A,B,C elements, we can construct *any* SiC polytype. Shown above are examples of the hexagonal polytypes 2H, 4H and 6H as they would be written in the Ramsdell classification scheme where the number indicates the layer and the letter indicates the Bravais lattice.[4] The 2H-SiC structure is equivalent to that of wurtzite and is composed of only elements A and B stacked as ABABAB. The 4H-SiC unit cell is two times longer, and the second half is twisted compared to 2H-SiC, resulting in ABCB stacking. The 6H-SiC cell is three times longer than that of 2H, and the stacking sequence is ABCACB. The cubic 3C-SiC (not shown) has ABC stacking.[5]

Physical properties

The different polytypes have widely ranging physical properties. 3C-SiC has the highest electron mobility and saturation velocity because of reduced phonon scattering resulting from the higher symmetry. The band gaps differ widely among the polytypes ranging from 2.3 eV for 3C-SiC to 3 eV in 6H SiC to 3.3 eV for 2H-SiC. In general, the greater the wurtzite component, the larger the band gap. Among the SiC polytypes, 6H is most easily prepared and best studied, while the 3C and 4H polytypes are attracting more attention for their superior electronic properties. The polytypism of SiC makes it nontrivial to grow single-phase material, but it also offers some potential advantages - if crystal growth methods can be developed sufficiently then heterojunctions of different SiC polytypes can be prepared and applied in electronic devices.[5]

Summary of polytypes

All symbols in the SiC structures have a specific meaning: The number 3 in 3C-SiC refers to the three-bilayer periodicity of the stacking (ABC) and the letter C denotes the cubic symmetry of the crystal. 3C-SiC is the only possible cubic polytype. The wurtzite ABAB... stacking sequence is denoted as 2H-SiC, indicating its two-bilayer stacking periodicity and hexagonal symmetry. This periodicity doubles and triples in 4H- and 6H-SiC polytypes. The family of rhombohedral polytypes is labeled R, for example, 15R-SiC.

Properties of major SiC polytypes[6][7][8][9][10] "Z" is number of atoms per unit cell, "SgNo" is space group number, *a* and *c* are lattice constants

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		

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External links

- A Brief History of Silicon Carbide (http://img.chem.ucl.ac.uk/www/kelly/moissanite.htm) Dr J F Kelly, University of London
- Material Safety Data Sheet (http://physchem.ox.ac.uk/MSDS/SI/silicon_carbide.html) for Silicon Carbide