Structure and energetics of elementary defects in 3C- and 4H-SiC

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related publications (since 2001):

Posselt, M., Gao, F., Weber, W. J., Belko, V.,
A comparative study of structure and energetics of elementary defects in 3C- and 4H-SiC,
J. Phys.: Condens. Matter 16 (2004) 1307

Gao, F., Posselt, M., Belko, V., Zhang, Y., Weber, W. J.,
Structures and energetics of defects: a comparative study of 3C- and 4H-SiC,
Nucl. Instr. Meth. B 218 (2004) 74

Gao, F., Weber, W. J., Posselt, M., Belko, V.,
Atomic computer simulations of defect migration in 3C and 4H-SiC,
Materials Science Forum 457-460 (2004) 457

Gao, F., Weber, W. J., Posselt, M., Belko, V.,
Atomistic study of intrinsic defect migration in 3C-SiC,
Phys. Rev. B 69 (2004) 245205

I. Introduction

SiC promising material for applications in power devices and high T electronics

selective electrical doping by ion implantation

but: ion-beam-induced defect production

understanding of defects and defect-related processes in SiC is therefore very important !!

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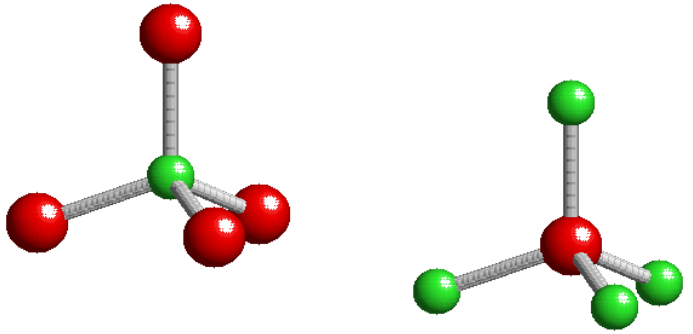
lattice structure

fourfold-coordinated **Si** and **C**



polytypism:

about 200 different SiC polytypes are known

identical nearest neighbors, but differences in the second, third ... neighbor shells

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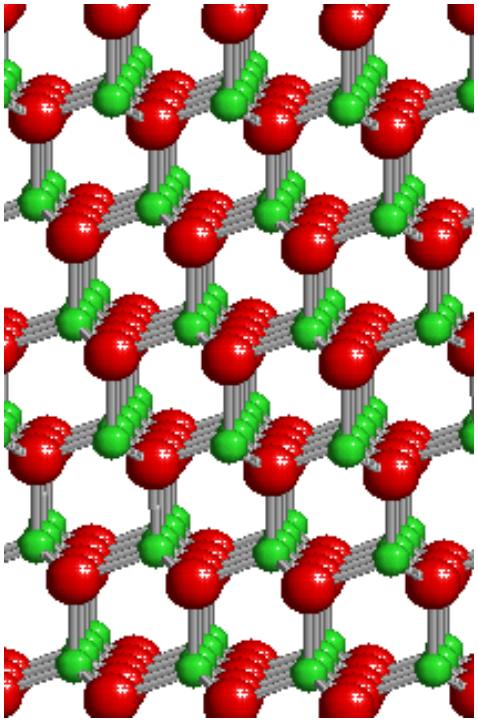
stack of layers of different CSi_4 tetrahedra,
along the c-axis

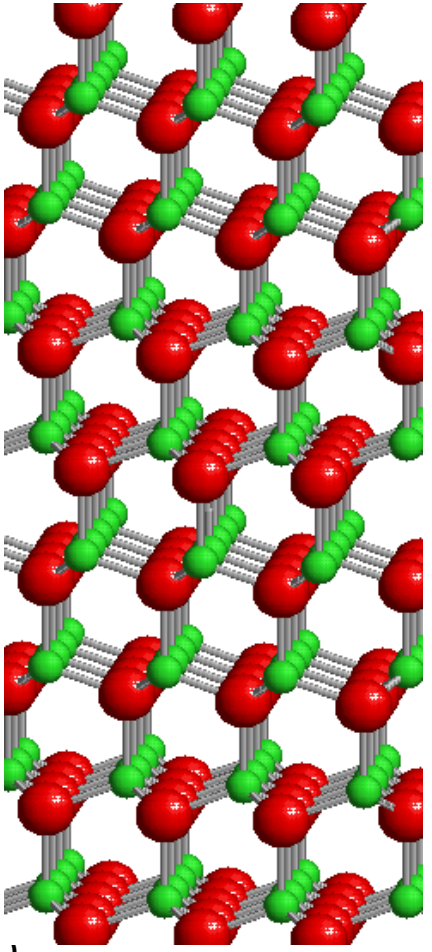
c-axis, [0001] *([111]$_c$)*

3C-SiC



T_3
T_2
T_1
T_3
T_2
T_1

4H-SiC



T_3'
T_1'
T_2
T_1
T_3'
T_1'
T_2
T_1

[-1100] *([-211]$_c$)*

[11-20] *([01-1]$_c$)*

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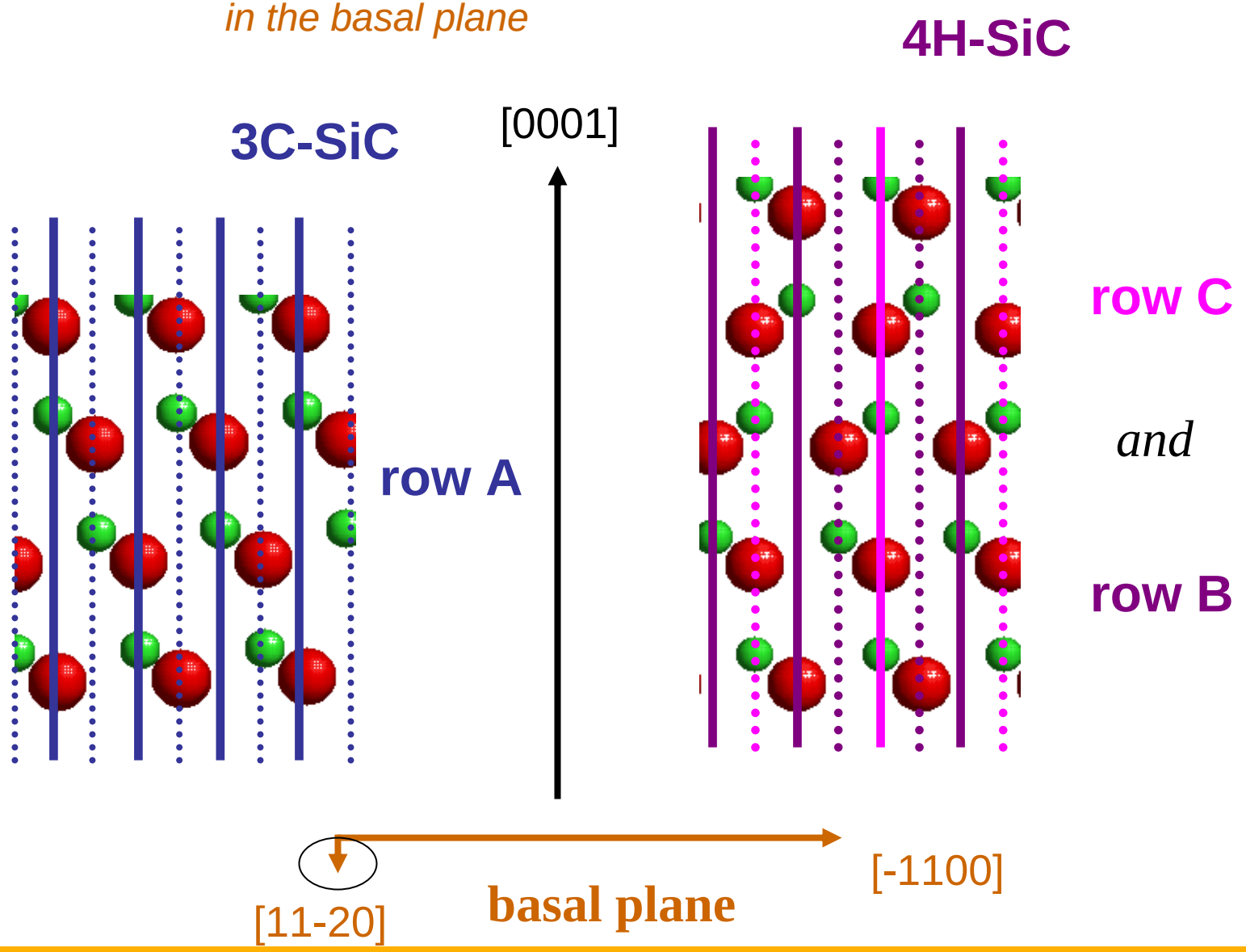
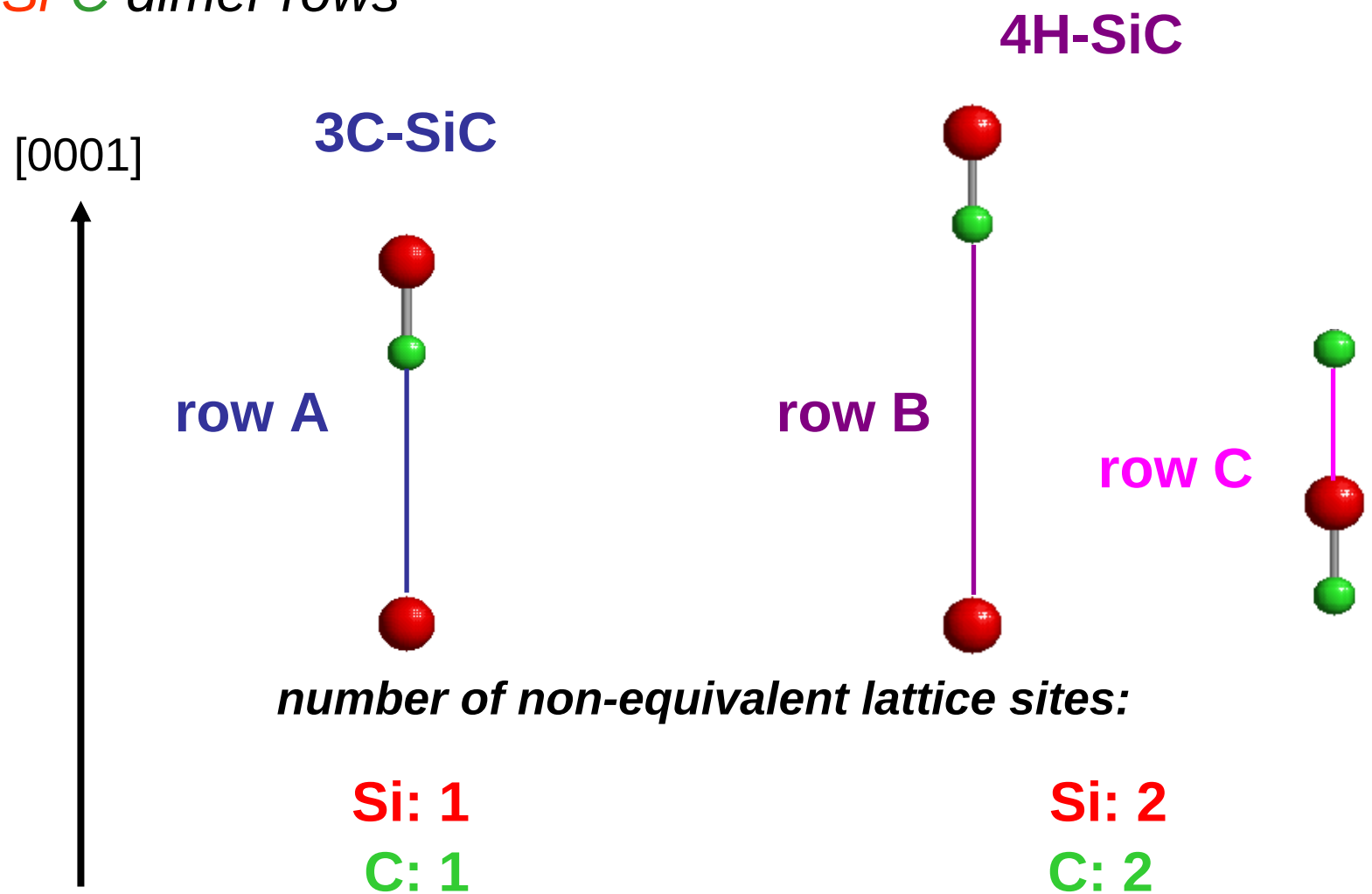
periodic arrangement of different Si-C dimer rows,
in the basal plane



Si-C dimer rows



number of non-equivalent lattice sites:

Si: 1
C: 1

Si: 2
C: 2

→ higher number of different defects configurations!!

SiC wafers available for technological applications:

4H and 6H

importance of investigations of defects in both polytypes!!

in the following: **4H,** 3C as reference material

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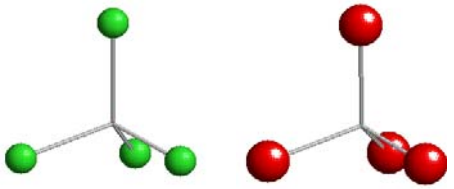
II. Classification of potential elementary defects based on symmetry considerations

non-equivalent on-site defects

3C-SiC | **4H-SiC**

vacancy

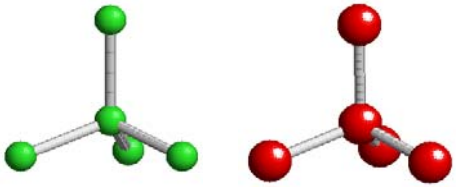
V_{Si}, V_C (2)



V_{Si}^{B}, V_{Si}^{C}, V_C^{B}, V_C^{C} **(4)**

antisite defect

Si_C, C_{Si} (2)

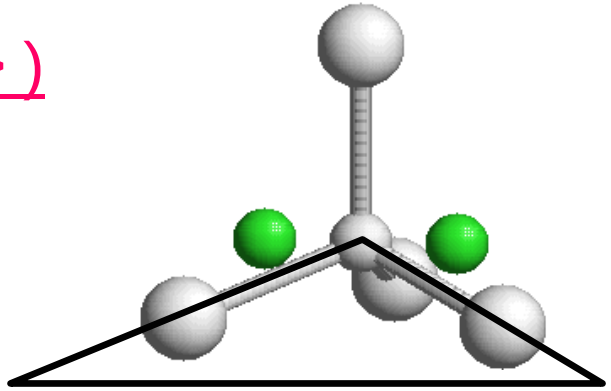


Si_C^{B}, Si_C^{C}, C_{Si}^{B}, C_{Si}^{C} **(4)**

dumbbell interstitial

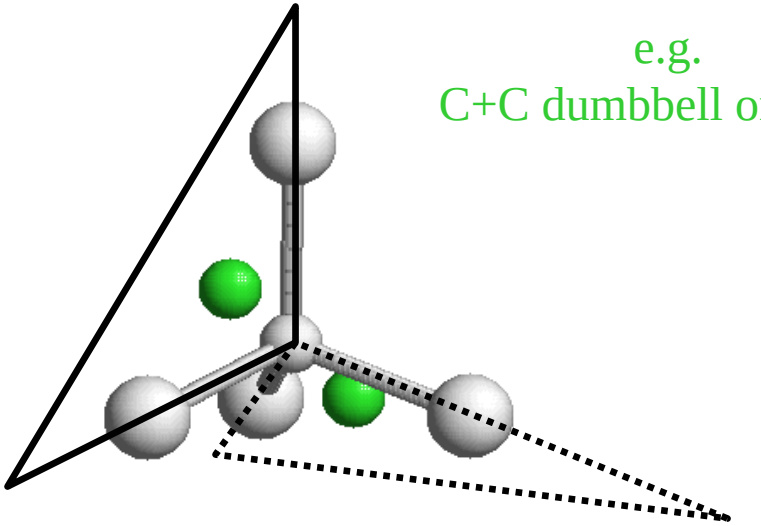
type 1 dumbbell (D1, <*110*>)

the dumbbell lies
in one of the six planes
formed by two C-Si bonds



type 2 dumbbell (D2, <*100*>)

the two atoms of the dumbbell
lie in perpendicular planes,
each plane is formed by two Si-C bonds



e.g.
C+C dumbbell on C-site

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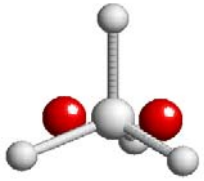
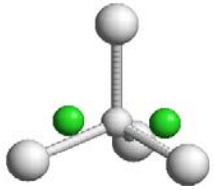
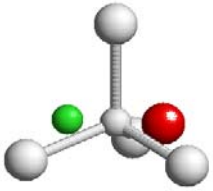
type 1 dumbbell



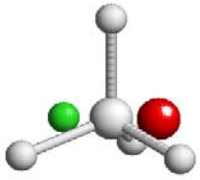
D1Si+Si
(Si+Si<110>)



D1C+C
(C+C<110>)



D1Si+C
(Si+C<110>)



D1C+Si
(C+Si<110>)

(4)

3C-SiC

4H-SiC

in basal plane (b): D1Si+Si^{b,B}, D1Si+Si^{b,C}

not in basal plane: D1Si+Si^{B}, D1Si+Si^{C}

D1C+C^{b,B},D1C+C^{b,C}

D1C+C^{B},D1C+C^{C}

D1Si+C^{b,B}, D1Si+C^{b,C}

two orientations (u, d) with respect to the c-axis:

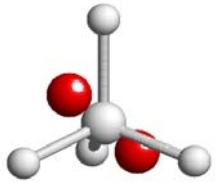
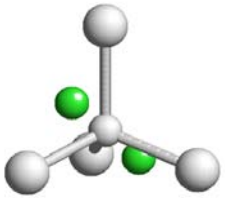
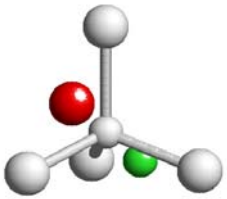
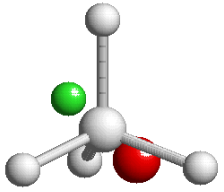
D1Si+C^{u,B}, D1Si+C^{d,B}, D1Si+C^{u,C}, D1Si+C^{d,C}

D1C+Si^{b,B}, D1C+Si^{b,C}

D1C+Si^{u,B}, D1C+Si^{d,B}, D1C+Si^{u,C}, D1C+Si^{d,C}

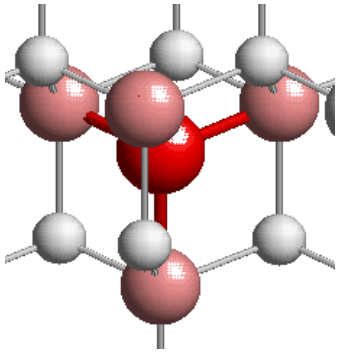
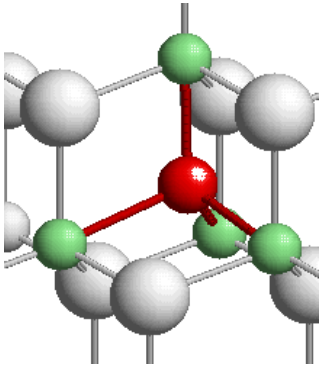
(20)

type 2 dumbbell

	3C-SiC	4H-SiC
	D2Si+Si *(Si+Si<100>)*	D2Si+Si^{B}, D2Si+Si^{C}
	D2C+C *(C+C<100>)*	D2C+C^{B}, D2C+C^{C}
	D2Si+C *(Si+C<100>)*	*two orientations (u,d) with respect to the c-axis:* D2Si+C^{u,B}, D2Si+C^{d,B} D2Si+C^{u,C}, D2Si+C^{d,C}
	D2C+Si *(C+Si<100>)*	D2C+Si^{u,B}, D2C+Si^{d,B} D2C+Si^{u,C}, D2C+Si^{d,C}
	(4)	**(12)**

non-equivalent elementary defects which are not related to lattice sites

tetrahedral interstitial

3C-SiC		4H-SiC
Si_{TSi}		Si_{TSi}
Si_{TC}		Si_{TC}
C_{TC}		C_{TC}
C_{TSi}		C_{TSi}
(4)		**(4)**

hexagonal interstitial

3C-SiC

Si_H, C_H

(2)

4H-SiC

Si_{HSi}, C_{HSi}, Si_{HC}, C_{HC}

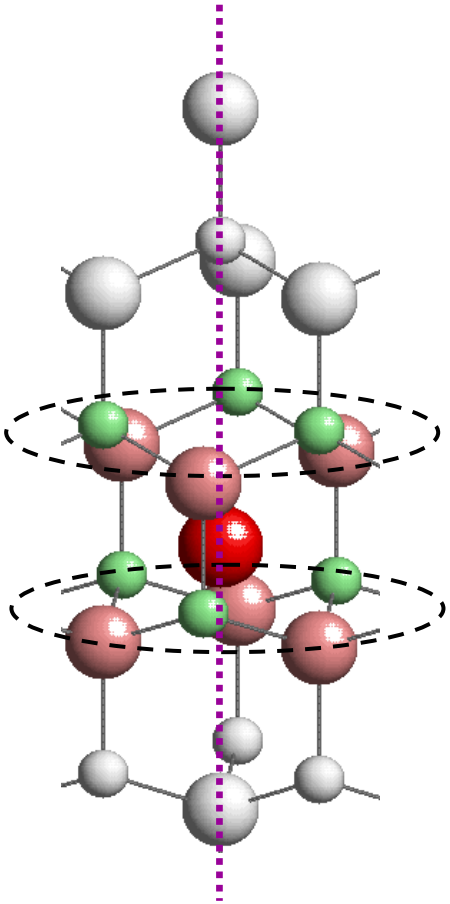
Si_H, C_H

(6)

interstitial between two Si_3C_3 hexagonal rings

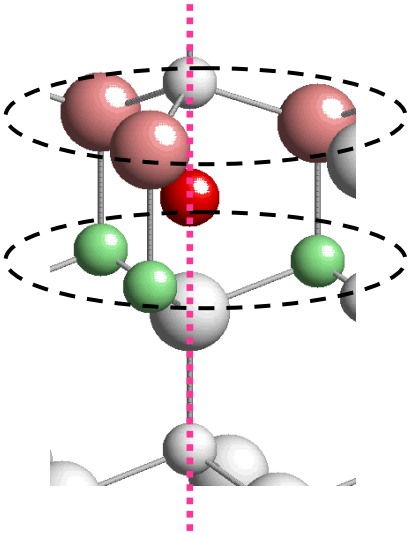
4H-SiC

Si_{HR}



row B (2)

interstitial between Si_3 and C_3 trigonal rings



C_{TR}

row C (2)

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III. MD study on stability, formation energy and structural details of the potential defects

Starting with the potential defect structure, **classical MD** simulations were performed to relax the SiC system at 0K, using a **rapid quenching** scheme. In the MD simulations, the **interatomic potential of Gao** and Weber [Nucl. Instrum. Methods in Phys. Res. B **191**, 504 (2002)] was employed.

Simulation cell: rectangular parallelepiped with x-, y-, z-directions parallel to [11-20], [-1100] and [0001], respectively; *periodic boundary conditions*, *1152 atoms (3C-SiC), 1920 atoms (4H-SiC)*

calculation of the defect formation energy

general definition via total energy differences:

$$E_D^f = E_D - n_{Si}\,\mu_{Si} - n_C\,\mu_C = E_D'^f - \tfrac{1}{2}\,(n_{Si} - n_C)\,\Delta\mu\ ,$$

with

$$E_D'^f = E_D - (n_{Si} + n_C)\,\mu_{SiC}^{bulk} - \tfrac{1}{2}\,(n_{Si} - n_C)\,(\mu_{Si}^{bulk} - \mu_C^{bulk})$$

$$\Delta\mu = (\mu_{Si} - \mu_{Si}^{bulk}) - (\mu_C - \mu_C^{bulk})$$

assumption: $\Delta\mu = 0$, i.e. $E_D^f = E_D'^f$ (stoichiometric case)

transformation to a relation containing differences of cohesive energies since in classical MD simulations only binding energies are considered

$$E_D'^f = E_{D,b} - (n_{Si} + n_C)\,E_{coh}^A(SiC) - \tfrac{1}{2}\,(n_{Si} - n_C)\,(E_{coh}^A(Si) - E_{coh}^A(C))$$

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results

most of the potential defects are found to be stable

the influence of polytypism depends on the complexity of the defect:

- small influence on compact defects and defects with nearly isotropic lattice deformations beyond the first nearest neighbors
- considerable influence on anisotropic defects with lattice deformations beyond the first nearest neighbor sphere

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defect energetics ($E_D{}^{\prime f}$ in eV)

vacancies and antisites	3C-SiC	4H-SiC	
	row A	***row B***	***row C***
V_{Si}	4.67	4.67	4.68
V_C	1.39	1.39	1.40
C_{Si}	4.43	4.43	4.44
Si_C	5.04	5.04	5.06

D1 dumbbells	**3C-SiC**	**4H-SiC**	
	row A	***row B***	***row C***
D1Si+Si^b	3.72	3.46	3.72
D1Si+Si		2.96	3.06
D1C+C^b	4.67	4.72	4.68
D1C+C		4.66	4.75
D1C+Si^b	5.32	5.34	5.32
D1C+Si^u		5.53	5.35
D1C+Si^d		5.30	5.59
D1Si+C^b	3.54*	not stable	3.40*
D1Si+C^u		3.01*	2.49*
D1Si+C^d		5.58*	6.03$^+$

D2 dumbbells	**3C-SiC**	**4H-SiC**	
	row A	***row B***	***row C***
D2Si+Si	4.15	4.16	4.18
D2C+C	4.41	4.41	4.43
D2C+Si^u	4.79	4.65	4.81
D2C+Si^d		4.78	4.81
D2Si+C^u	6.06$^+$	4.18*	2.83$^+$
D2Si+C^d		6.07$^+$	6.11$^+$

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defect energetics ($E_D{}^{\prime f}$ in eV)

	3C-SiC	4H-SiC	
	row A	***row B***	***row C***
tetrahedral interstitials			
Si_{TSi}	5.39	5.38	
Si_{TC}	2.60	2.60	
C_{TSi}	5.69	5.69	
C_{TC}	5.38	5.37	
hexagonal interstitials			
Si_H	not stable	not stable	
Si_{HSi}		not stable	
Si_{HC}		not stable	
C_H	5.15	5.15	
C_{HSi}		5.15	
C_{HC}		5.15	
interstitials between two hexagonal Si_3C_3 rings			
Si_{HR}		3.39	
C_{HR}		4.85	
interstitials between Si_3 and C_3 trigonal rings			
Si_{TR}			not stable
C_{TR}			6.26

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IV. Summary

- most of the potential elementary defects are stable

- number of non-equivalent defects in 4H-SiC is much higher than in 3C-SiC

→ *consequences for modeling of defect migration*

- *many compact defects in 4H-SiC have similar formation energy and structure like the corresponding defects in 3C-SiC*

- *differences are obtained for more complex defects with large lattice deformations*