First-principles and empirical potential simulation study of intrinsic and carbon-related defects in silicon

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Motivation & Outline

Ion beam synthesis (IBS) of epitaxial single crystalline 3C-SiC

- **Implantation**
  
  Stoichiometric dose | 180 keV | 500 °C
  
  ⇒ Epitaxial 3C-SiC layer & precipitates

- **Annealing**
  
  10 h at 1250 °C
  
  ⇒ Homogeneous 3C-SiC layer

  3C-SiC precipitation not yet fully understood

Outline

- Assumed SiC precipitation mechanisms / Controversy
- Utilized simulation techniques
- C and Si self-interstitial point defects in silicon
- Silicon carbide precipitation simulations
Supposed precipitation mechanism of SiC in Si

Silicon and SiC lattice structure

Silicon
Si | Si
\( a = 5.429 \text{ Å} \)
\( \rho_{\text{Si}}^* = 100\% \)

Silicon carbide
Si | C
\( a = 4.359 \text{ Å} \)
\( \rho_{\text{Si}}^* = 97\% \)

C-Si dimers (dumbbells) on Si lattice sites

Agglomeration of C-Si dumbbells ⇒ dark contrasts

Precipitation of 3C-SiC in Si ⇒ Moiré fringes & release of Si self-interstitials

(\( h k l \) planes match)

Distance \( r = 2-4 \text{ nm} \)

4\( a_{\text{Si}} = 5a_{\text{SiC}} \)
Supposed precipitation mechanism of SiC in Si

### Controversial findings

- **High-temperature implantation** /Nejim et al./
  - Substitutionally incorporated C on regular Si lattice sites
  - $\text{Si}_i$ reacting with further C in cleared volume

- **Annealing behavior** /Serre et al./
  - Room temperature implantation $\rightarrow$ high C diffusion
  - Elevated temperature implantation $\rightarrow$ no C redistribution
  $\Rightarrow$ mobile $C_i$ opposed to stable $C_{\text{sub}}$ configurations

- **Strained Si$_{1-y}$C$_y$/Si heterostructures** /Strane et al./Guedj et al./
  - Initial coherent SiC structures (tensile strain)
  - Incoherent SiC nanocrystals (strain relaxation)

$4a_{\text{Si}} = 5a_{\text{SiC}}$

$C_{\text{sub}} \quad \text{vs} \quad C_i$
Utilized computational methods

**Molecular dynamics (MD)**

<table>
<thead>
<tr>
<th>System of $N$ particles</th>
<th>$N = 5832 \pm 1$ (Defects), $N = 238328 + 6000$ (Precipitation)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phase space propagation</td>
<td>Velocity Verlet</td>
</tr>
<tr>
<td>Analytical interaction potential</td>
<td>Tersoff-like short-range, bond order potential (Erhart/Albe)</td>
</tr>
<tr>
<td></td>
<td>$E = \frac{1}{2} \sum_{i \neq j} V_{ij}$, $V_{ij} = f_C(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})]$</td>
</tr>
<tr>
<td>Observables: time/ensemble averages</td>
<td>NpT (isothermal-isobaric)</td>
</tr>
</tbody>
</table>

**Density functional theory (DFT)**

- Hohenberg-Kohn theorem:
  $\Psi_0(r_1, r_2, \ldots, r_N) = \Psi[n_0(r)], E_0 = E[n_0]$
- Kohn-Sham approach:
  Single-particle effective theory

- Code: **vasp**
- Plane wave basis set | $E_{\text{cut}} = 300$ eV
- Ultrasoft pseudopotential
- Exchange & correlation: GGA
- Brillouin zone sampling: Γ-point
- Supercell: $N = 216 \pm 2$

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{eff}}(r) - \epsilon_i \right] \Phi_i(r) = 0
\]

\[
n(r) = \sum_i |\Phi_i(r)|^2
\]

\[
V_{\text{eff}}(r) = V_{\text{ext}}(r) + \int \frac{e^2 n(r')}{|r - r'|} d^3r' + V_{XC}[n(r)]
\]
Point defects & defect migration

Defect structure

- Creation of c-Si simulation volume
- Periodic boundary conditions
- $T = 0$ K, $p = 0$ bar

Insertion of interstitial C/Si atoms

Relaxation / structural energy minimization

Defect formation energy

$$E_f = E - \sum_i N_i \mu_i$$

Binding energy

$$E_b = E_f^{\text{comb}} - E_f^{1\text{st}} - E_f^{2\text{nd}}$$

$E_b < 0$: energetically favorable configuration
$E_b \rightarrow 0$: non-interacting, isolated defects

Migration barrier

- Displace diffusing atom
- Constrain relaxation of (diffusing) atoms
- Record configurational energy
## C interstitial point defects in silicon

<table>
<thead>
<tr>
<th>$E_f$ [eV]</th>
<th>T</th>
<th>H</th>
<th>$\langle 100 \rangle$ DB</th>
<th>$\langle 110 \rangle$ DB</th>
<th>S</th>
<th>B</th>
<th>$C_{sub}$ &amp; $Si_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>VASP</td>
<td>unstable</td>
<td>unstable</td>
<td>3.72</td>
<td>4.16</td>
<td>1.95</td>
<td>4.66</td>
<td>4.17</td>
</tr>
<tr>
<td>Erhart/Albe</td>
<td>6.09</td>
<td>9.05*</td>
<td>3.88</td>
<td>5.18</td>
<td>0.75</td>
<td>5.59*</td>
<td>4.43</td>
</tr>
</tbody>
</table>

### Hexagonal

$E_f^* = 9.05$ eV

$\langle 100 \rangle$ $E_f = 3.88$ eV

### Bond-centered

$E_f^* = 5.59$ eV

$\langle 110 \rangle$ dumbbell $E_f = 5.18$ eV

$\Rightarrow$ Substitutional

$\Rightarrow$ Tetrahedral
**C interstitial migration**

### First-principles

$[00\bar{1}] \rightarrow [0\bar{1}0]$

$\Delta E = 0.9 \text{ eV} \mid \text{Experimental values: } 0.70–0.87 \text{ eV}$

$\Rightarrow \text{Migration mechanism identified!}$

Note: Change in orientation

### Empirical potential

$[00\bar{1}] \rightarrow [110] \rightarrow [0\bar{1}0]$

- Transition involving $[110]$ DB (instability of BC configuration)
- $\Delta E \approx 2.2 \text{ eV} \ & 0.9 \text{ eV}$
- $2.4 - 3.4$ times higher than ab initio result
- After all: Change of the DB orientation

Drastically overestimated diffusion barrier
# Defect combinations — ab inito

## Summary of combinations

<table>
<thead>
<tr>
<th>$E_b$ [eV]</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0 0 1]</td>
<td>-0.08</td>
<td>-1.15</td>
<td>-0.08</td>
<td>0.04</td>
<td>-1.66</td>
<td>-0.19</td>
</tr>
<tr>
<td>[0 0 1]</td>
<td>0.34</td>
<td>0.004</td>
<td>-2.05</td>
<td>0.26</td>
<td>-1.53</td>
<td>-0.19</td>
</tr>
<tr>
<td>[0 1 0]</td>
<td>-2.39</td>
<td>-0.17</td>
<td>-0.10</td>
<td>-0.27</td>
<td>-1.88</td>
<td>-0.05</td>
</tr>
<tr>
<td>[0 1 0]</td>
<td>-2.25</td>
<td>-1.90</td>
<td>-2.25</td>
<td>-0.12</td>
<td>-1.38</td>
<td>-0.06</td>
</tr>
<tr>
<td>[1 0 0]</td>
<td>-2.39</td>
<td>-0.36</td>
<td>-2.25</td>
<td>-0.12</td>
<td>-1.88</td>
<td>-0.05</td>
</tr>
<tr>
<td>[1 0 0]</td>
<td>-2.25</td>
<td>-2.16</td>
<td>-0.10</td>
<td>-0.27</td>
<td>-1.38</td>
<td>-0.06</td>
</tr>
<tr>
<td>$C_{sub}$</td>
<td>0.26</td>
<td>-0.51</td>
<td>-0.93</td>
<td>-0.15</td>
<td>0.49</td>
<td>-0.05</td>
</tr>
<tr>
<td>Vacancy</td>
<td>-5.39</td>
<td>-0.59</td>
<td>-3.14</td>
<td>-0.54</td>
<td>-0.50</td>
<td>-0.31</td>
</tr>
</tbody>
</table>

## Combinations of $\langle 100 \rangle$-type interstitials

- $C_i$ agglomeration energetically favorable
- Reduction of strain
- Capture radius exceeding 1 nm
- Disappearance of attractive forces between two lowest separations.

$C_i$ agglomeration / no C clustering
Defect combinations of C-Si dimers and vacancies

$V$ at 2: $E_b = -0.59$ eV

\[ E_b = -0.59 \text{ eV} \]

$V$ at 3, $E_b = -3.14$ eV

**IBS: Impinging C creates V & far away $Si_i$**

- Low migration barrier towards $C_{sub}$
- High barrier for reverse process

**High probability of stable $C_{sub}$ configuration**

```
[0 0 1]  [1 0 0]
```

```
0 20 40 60 80 100
```

\[ \Delta E \text{ [eV]} \]

- Displacement [%]

```
[0 0 1]  [1 0 0]
```

\[ \Delta E \text{ [eV]} \]

- Displacement [%]

\[ \Delta E \text{ [eV]} \]

- Displacement [%]
Combinations of substitutional C and Si self-interstitials

$C_{\text{sub}} - Si_i \langle 110 \rangle$ interaction
- Most favorable: $C_{\text{sub}}$ along $\langle 110 \rangle$ chain of $Si_i$
- Less favorable than ground-state $C_i \langle 100 \rangle$ DB
- Interaction drops quickly to zero → low capture radius

Transition from the ground state
- Low transition barrier
- Barrier smaller than $C_i$ migration barrier
- Low $Si_i$ migration barrier (0.67 eV) → Separation of $C_{\text{sub}}$ & $Si_i$ most probable

$C_{\text{sub}}$ & $Si_i$ instead of thermodynamic ground state

IBS — process far from equilibrium
Combinations of substitutional C and Si self-interstitials

$C_{\text{sub}} - Si_i \langle 1\ 1\ 0 \rangle$ interaction
- Most favorable: $C_{\text{sub}}$ along $\langle 1\ 1\ 0 \rangle$ chain of $Si_i$
- Less favorable than ground-state $C_i \langle 1\ 0\ 0 \rangle$ DB

Transition from the ground state
- Low transition barrier
- Barrier smaller than $C_i$ migration barrier
- Low $Si_i$ migration barrier (0.67 eV)

$C_{\text{sub}} & Si_i$ instead of thermodynamic ground state

IBS — process far from equilibrium
Silicon carbide precipitation simulations

Procedure

- Create c-Si volume
- Periodic boundary conditions
- Set requested $T$ and $p = 0$ bar
- Equilibration of $E_{\text{kin}}$ and $E_{\text{pot}}$

Insertion of C atoms at constant T
- total simulation volume
- volume of minimal SiC precipitate size
- volume containing Si atoms to form a minimal precipitate

Run for 100 ps followed by cooling down to 20°C

Note
- Amount of C atoms: 6000
  ($r_{\text{prec}} \approx 3.1$ nm, IBS: 2–4 nm)
- Simulation volume: $31^3$ Si unit cells
  (238328 Si atoms)

Restricted to classical potential calculations
→ Low C diffusion / overestimated barrier
→ Consider $V_2$ and $V_3$
Silicon carbide precipitation simulations

Temperature as used in IBS (450 °C)

$C_i \langle 1 0 0 \rangle$ dumbbell dominated structure

Formation of $C_i$ DBs

No agglomeration / precipitation

Limitations:
- Time scale problem of MD
  ⇒ slow phase space propagation
- Short range potential
  ⇒ overestimated diffusion barrier

Increased temperatures

$C_{sub}$ dominated structure

$\text{Si-}C_{sub}\text{-Si along }\langle 1 1 0 \rangle$

$C_{sub}\text{-Si-}C_{sub}$ & nearby $Si_i$

Conclusions:
- Stretched coherent SiC structures
  ⇒ $C_{sub}$ involved in precipitation mechanism
- Reduction in strain by $Si_i$
Summary and Conclusions

Summary

• First-principles investigation of defect combinations and mobilities in Si

• Empirical potential MD simulations on SiC precipitation in Si

Conclusions on SiC precipitation

\[ C_i \leftarrow \text{vs} \rightarrow C_{\text{sub}} \]

• \( C_{\text{sub}} \) involved in the precipitation mechanism

• Role of the \( \text{Si}_i \)
  - Vehicle to rearrange \( C_{\text{sub}} \leftarrow [C_{\text{sub}} \& \text{Si}_i \leftrightarrow C_i] \)
  - Building block for surrounding Si host & further SiC
  - Strain compensation …
  - \( \ldots \)Si/SiC interface
  - \( \ldots \)within stretched coherent SiC structure

Further conclusions

• High T \( \leftrightarrow \) IBS conditions far from equilibrium
Acknowledgements

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• Prof. B. Stritzker

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• Prof. J. Lindner
• Prof. G. Schmidt
• Dr. E. Rauls

Thank you for your attention!
### Polytypes of SiC

<table>
<thead>
<tr>
<th></th>
<th>3C-SiC</th>
<th>4H-SiC</th>
<th>6H-SiC</th>
<th>Si</th>
<th>GaN</th>
<th>Diamond</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hardness [Mohs]</td>
<td>—— 9.6</td>
<td>——</td>
<td>6.5</td>
<td>——</td>
<td>——</td>
<td>10</td>
</tr>
<tr>
<td>Band gap [eV]</td>
<td>2.36</td>
<td>3.23</td>
<td>3.03</td>
<td>1.12</td>
<td>3.39</td>
<td>5.5</td>
</tr>
<tr>
<td>Break down field [$10^6$ V/cm]</td>
<td><strong>4</strong></td>
<td><strong>3</strong></td>
<td><strong>3.2</strong></td>
<td><strong>0.6</strong></td>
<td><strong>5</strong></td>
<td><strong>10</strong></td>
</tr>
<tr>
<td>Saturation drift velocity [$10^7$ cm/s]</td>
<td><strong>2.5</strong></td>
<td>2.0</td>
<td>2.0</td>
<td>1</td>
<td>2.7</td>
<td>2.7</td>
</tr>
<tr>
<td>Electron mobility [cm$^2$/Vs]</td>
<td>800</td>
<td>900</td>
<td>400</td>
<td>1100</td>
<td>900</td>
<td>2200</td>
</tr>
<tr>
<td>Hole mobility [cm$^2$/Vs]</td>
<td><strong>320</strong></td>
<td>120</td>
<td>90</td>
<td>420</td>
<td>150</td>
<td>1600</td>
</tr>
<tr>
<td>Thermal conductivity [W/cmK]</td>
<td>5.0</td>
<td>4.9</td>
<td>4.9</td>
<td>1.5</td>
<td><strong>1.3</strong></td>
<td>22</td>
</tr>
</tbody>
</table>
IBS of epitaxial single crystalline 3C-SiC

- **Implantation step 1**
  Almost stoichiometric dose | 180 keV | 500 °C
  ⇒ Epitaxial 3C-SiC layer & precipitates

- **Implantation step 2**
  Low remaining amount of dose | 180 keV | 250 °C
  ⇒ Destruction/Amorphization of precipitates at layer interface

- **Annealing**
  10 h at 1250 °C
  ⇒ Homogeneous 3C-SiC layer with sharp interfaces

3C-SiC precipitation not yet fully understood

XTEM: single crystalline 3C-SiC in Si(1 0 0)
Si self-interstitial point defects in silicon

<table>
<thead>
<tr>
<th>$E_f$ [eV]</th>
<th>⟨1 1 0⟩ DB</th>
<th>H</th>
<th>T</th>
<th>⟨1 0 0⟩ DB</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td>VASP</td>
<td>3.39</td>
<td>3.42</td>
<td>3.77</td>
<td>4.41</td>
<td>3.63</td>
</tr>
<tr>
<td>Erhart/Albe</td>
<td>4.39</td>
<td>4.48*</td>
<td>3.40</td>
<td>5.42</td>
<td>3.13</td>
</tr>
</tbody>
</table>

Vacancy

 ⟨110⟩ DB

 ⟨100⟩ DB

 Tetrahedral

Hexagonal

$E_f^* = 4.48$ eV

$E_f = 3.96$ eV

nearby T $\rightarrow$ T

Displacement [%]
C-Si dimer & bond-centered interstitial configuration

C $\langle 1\ 0\ 0 \rangle$ DB interstitial

<table>
<thead>
<tr>
<th>Erhart/Albe</th>
<th>VASP</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="C-Si dimer &amp; bond-centered interstitial configuration" /></td>
<td><img src="image2" alt="C-Si dimer &amp; bond-centered interstitial configuration" /></td>
</tr>
</tbody>
</table>

Si-C-Si bond angle $\rightarrow 180^\circ$  
$\Rightarrow sp$ hybridization

Si-Si-Si bond angle $\rightarrow 120^\circ$  
$\Rightarrow sp^2$ hybridization

Bond-centered interstitial

- Linear Si-C-Si bond
- Si: one C & 3 Si neighbours
- Spin polarized calculations
- No saddle point!  
  Real local minimum!

<table>
<thead>
<tr>
<th>Si</th>
<th>MO</th>
<th>C</th>
<th>MO</th>
<th>Si</th>
</tr>
</thead>
<tbody>
<tr>
<td>$sp^3$</td>
<td></td>
<td>$sp$</td>
<td></td>
<td>$sp^3$</td>
</tr>
</tbody>
</table>

$\uparrow \uparrow \uparrow$  
$\sigma_{ab}$

$\uparrow \downarrow \uparrow$  
$\sigma_b$

Charge density

- Spin up
- Spin down
- Resulting spin up
- Si atoms
- C atom

Charge density isosurface
C interstitial migration — ab initio

\[ [0 0 \overline{1}] \rightarrow [0 0 1] \]

Symmetry:
⇒ Sufficient to consider \([0 0 \overline{1}]\) to BC transition
⇒ Migration barrier to reach BC \(\Delta E = 1.2\ eV\)

\[ [0 0 \overline{1}] \rightarrow [0 \overline{1} 0] \]

\(\Delta E = 0.9\ eV\) | Experimental values: 0.70–0.87 eV
⇒ Migration mechanism identified!
Note: Change in orientation
C interstitial migration — analytical potential

BC to $[0\ 0\ 1]$ transition

- Lowermost migration barrier
- $\Delta E \approx 2.2\ eV$
- 2.4 times higher than ab initio result
- Different pathway

Transition involving a $\langle 1\ 1\ 0 \rangle$ configuration

- Bond-centered configuration unstable
  $\rightarrow C_i \langle 1\ 1\ 0 \rangle$ dumbbell
- Minimum of the $[0\ 0\ 1]$ to $[0\ 1\ 0]$ transition
  $\rightarrow C_i \langle 1\ 1\ 0 \rangle$ DB

- $\Delta E \approx 2.2\ eV \ & \ 0.9\ eV$
- 2.4 – 3.4 times higher than ab initio result
- After all: Change of the DB orientation

Drastically overestimated diffusion barrier
Silicon carbide precipitation simulations at 450 °C as in IBS

Low C concentration — $V_1$

$C_i \langle 1 0 0 \rangle$ dumbbell dominated structure
- Si-C bumps around 0.19 nm
- C-C peak at 0.31 nm (expected in 3C-SiC): concatenated differently oriented $C_i$ DBs
- Si-Si NN distance stretched to 0.3 nm

Formation of $C_i$ dumbbells
$C$ atoms separated as expected in 3C-SiC

High C concentration — $V_2/V_3$

- High amount of strongly bound C-C bonds
- Increased defect & damage density
  → Arrangements hard to categorize and trace
- Only short range order observable

Amorphous SiC-like phase

Formation of 3C-SiC fails to appear

$V_1$: Formation of $C_i$ indeed occurs
Agglomeration not observed

$V_{2,3}$: (not expected at 450 °C)
No rearrangement/transition into 3C-SiC
Increased temperature simulations — $V_1$

Si-C bonds:
- Vanishing cut-off artifact (above 1650 °C)
- Structural change: $C_i \langle 1 0 0 \rangle$ DB $\rightarrow C_{sub}$

Si-Si bonds: Si-C$_{sub}$-Si along $\langle 1 1 0 \rangle$ ($\rightarrow 0.325$ nm)

C-C bonds:
- C-C next neighbour pairs reduced (mandatory)
- Peak at 0.3 nm slightly shifted
  $\rightarrow C_i$ combinations (dashed arrows)
  $\uparrow C_i \langle 1 0 0 \rangle$ & $C_{sub}$ combinations ($\uparrow$)
  $\uparrow C_i$ pure $C_{sub}$ combinations ($\downarrow$)
Range $[\downarrow-\uparrow]$: $C_{sub} \& C_{sub}$ with nearby Si$_i$
Increased temperature simulations at high C concentration

0.186 nm: Si-C pairs ↑ (as expected in 3C-SiC)
0.282 nm: Si-C-C
≈0.35 nm: C-Si-Si

- Decreasing cut-off artifact
- Amorphous SiC-like phase remains
- High amount of damage & alignment to c-Si host matrix lost
- Slightly sharper peaks ⇒ indicate slight acceleration of dynamics due to temperature

0.15 nm: C-C pairs ↑ (as expected in graphite/diamond)
0.252 nm: C-C-C (2nd NN for diamond)
0.31 nm: shifted towards 0.317 nm → C-Si-C

High C & small V & short t ⇒ Slow structural evolution due to strong C-C bonds ⇐ High C & low T implants
Long time scale simulations at maximum temperature

Differences

- Temperature set to $0.95 \cdot T_m$
- Cubic insertion volume $\Rightarrow$ spherical insertion volume
- Amount of C atoms: $6000 \rightarrow 5500 \Leftrightarrow r_{\text{prec}} = 0.3$ nm
- Simulation volume: 21 unit cells of c-Si in each direction

Low C concentration, Si-C

![Graph of g(r) for Si-C with peaks at t = 0.6 ns, 2.7 ns, and 4.8 ns at r = 0.1 to 0.6 nm.]

Sharper peaks!

Low C concentration, C-C

![Graph of g(r) for C-C with peaks at t = 0.6 ns, 2.7 ns, and 4.8 ns at r = 0.1 to 0.6 nm.]

Sharper peaks!

No C agglomeration!

High C concentration

![Graph of g(r) for C-C with peaks at t = 0.7 ns, 3.7 ns, and 6.1 ns at r = 0.1 to 0.6 nm.]

No significant changes

iC-Si-Si $\uparrow$

C-Si-C $\downarrow$

Long time scales and high temperatures most probably not sufficient enough!
Investigation of a silicon carbide precipitate in silicon

\[
\frac{8}{a_{\text{Si}}^3} \left( \frac{4}{3} \pi x^3 \right) + \frac{4}{y^3} \frac{4}{3} \pi x^3 = 21^3 \cdot 8
\]

\[
\Rightarrow \quad \frac{8}{a_{\text{Si}}^3} \frac{4}{3} \pi x^3 = 5500 \Rightarrow x = \left( \frac{5500 \cdot 3}{32 \pi} \right)^{1/3} a_{\text{Si}}
\]

\[
y = \left( \frac{1}{2} \right)^{1/3} a_{\text{Si}}
\]

Construction
- Simulation volume: 21\(^3\) unit cells of c-Si
- Spherical topotactically aligned precipitate \(r = 3.0\) nm \(\Rightarrow \approx 5500\) C atoms
- Create c-Si but skipped inside sphere of radius \(x\)
- Create 3C-SiC inside sphere of radius \(x\) and lattice constant \(y\)
- Strong coupling to heat bath \((T = 20^\circ\text{C})\)

Results
- Slight increase of c-Si lattice constant!
- C-C peaks (imply same distanced Si-Si peaks)
  - New peak at 0.307 nm: 2\(^{\text{nd}}\) NN in 3C-SiC
  - Bumps (\(\downarrow\)): 4\(^{\text{th}}\) and 6\(^{\text{th}}\) NN
- 3C-SiC lattice constant: 4.34 Å (bulk: 4.36 Å) \(\Rightarrow\) compressed precipitate
- Interface tension:
  - 20.15 eV/nm\(^2\) or \(3.23 \times 10^{-4}\) J/cm\(^2\)
  - (literature: \(2 - 8 \times 10^{-4}\) J/cm\(^2\))
Investigation of a silicon carbide precipitate in silicon

Appended annealing steps

- artificially constructed interface
  → allow for rearrangement of interface atoms
- check SiC stability

Temperature schedule

- rapidly heat up structure up to 2050 °C (75 K/ps)
- slow heating up to $1.2 \cdot T_m = 2940$ K by 1 K/ps
  → melting at around 2840 K
- cooling down structure at 100 % $T_m$ (1 K/ps)
  → no energetically more favorable structure
## DFT parameters

Equilibrium lattice constants and cohesive energies

<table>
<thead>
<tr>
<th></th>
<th>USPP, LDA</th>
<th>USPP, GGA</th>
<th>PAW, LDA</th>
<th>PAW, GGA</th>
<th>Exp.</th>
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<tbody>
<tr>
<td>Si (dia)</td>
<td>$a$ [Å]</td>
<td>5.389</td>
<td>5.455</td>
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<tr>
<td></td>
<td>$\Delta a$ [%]</td>
<td>0.7 %</td>
<td>0.5 %</td>
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<tr>
<td></td>
<td>$E_{coh}$ [eV]</td>
<td>-5.277</td>
<td>-4.591</td>
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<tr>
<td></td>
<td>$\Delta E$ [%]</td>
<td>14.0 %</td>
<td>0.8 %</td>
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<tr>
<td>C (dia)</td>
<td>$a$ [Å]</td>
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<td>3.567</td>
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<tr>
<td></td>
<td>$\Delta a$ [%]</td>
<td>1.1 %</td>
<td>0.01 %</td>
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<tr>
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<td>$E_{coh}$ [eV]</td>
<td>-8.812</td>
<td>-7.703</td>
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<td>$\Delta E$ [%]</td>
<td>19.5 %</td>
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<tr>
<td>3C-SiC</td>
<td>$a$ [Å]</td>
<td>4.319</td>
<td>4.370</td>
<td>4.330</td>
<td>4.379</td>
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<td>$\Delta a$ [%]</td>
<td>0.9 %</td>
<td>0.3 %</td>
<td>0.7 %</td>
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</tr>
<tr>
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<td>$\Delta E$ [%]</td>
<td>15.4 %</td>
<td>1.4 %</td>
<td>16.3 %</td>
<td>2.4 %</td>
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<table>
<thead>
<tr>
<th></th>
<th>Si (dia)</th>
<th>C (dia)</th>
<th>3C-SiC</th>
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</thead>
<tbody>
<tr>
<td>$a$ [Å]</td>
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<td>4.365</td>
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<td>0.1</td>
<td>0.1</td>
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<td>$E_{coh}$ [eV]</td>
<td>-4.577</td>
<td>-7.695</td>
<td>-6.419</td>
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<tr>
<td>$\Delta E$ [%]</td>
<td>1.1</td>
<td>4.4</td>
<td>1.2</td>
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← entire parameter set
DFT parameters

Lattice constants with respect to the PW cut-off energy

Defect formation energy with respect to the size of the supercell