Molecular dynamics simulation study of the silicon carbide precipitation process

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Motivation / Introduction

Reasons for understanding the SiC precipitation process:

- 3C-SiC wide band gap semiconductor formation
- Strained Si (no precipitation wanted!)

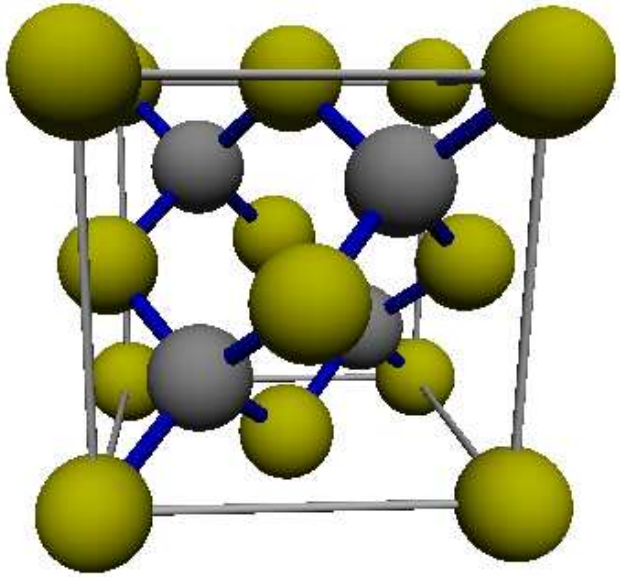
Si / 3C-SiC facts:

- Unit cell:
  - fcc +
  - fcc shifted 1/4 of volume diagonal
- Lattice constants:

$$4a_{Si} \approx 5a_{SiC}$$

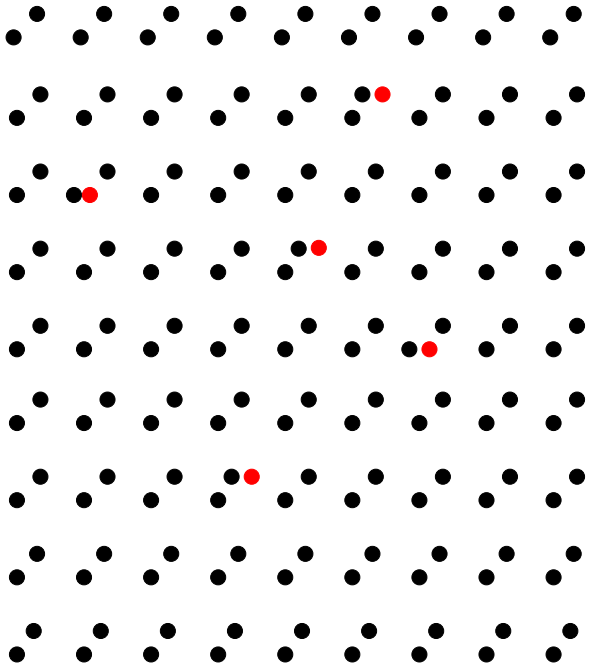
- Silicon density:

$$\frac{n_{SiC}}{n_{Si}} = 97,66\,\%$$

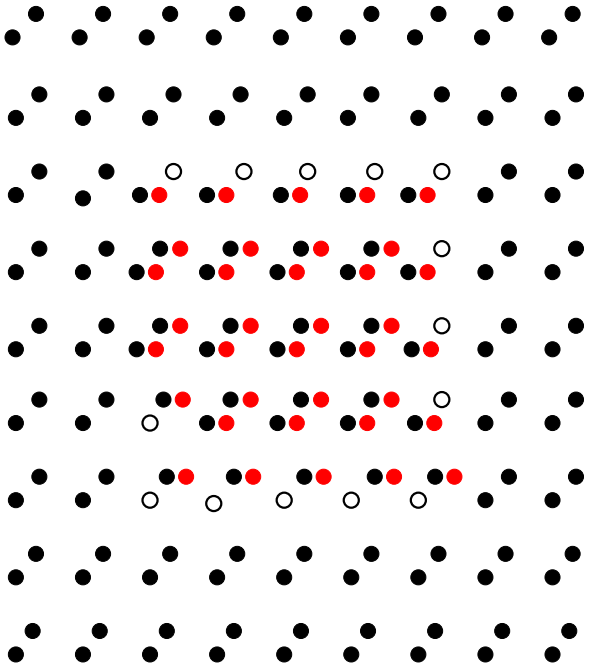


Motivation / Introduction

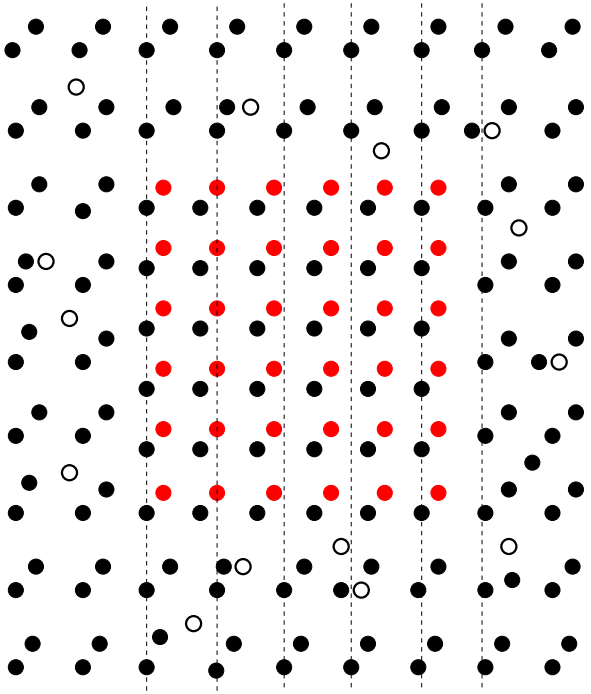
Supposed conversion mechanism of heavily carbon doped Si into SiC:



Formation of C-Si dumbbells on regular c-Si lattice sites



Agglomeration into large clusters (embryos)



Precipitation of 3C-SiC + Creation of interstitials

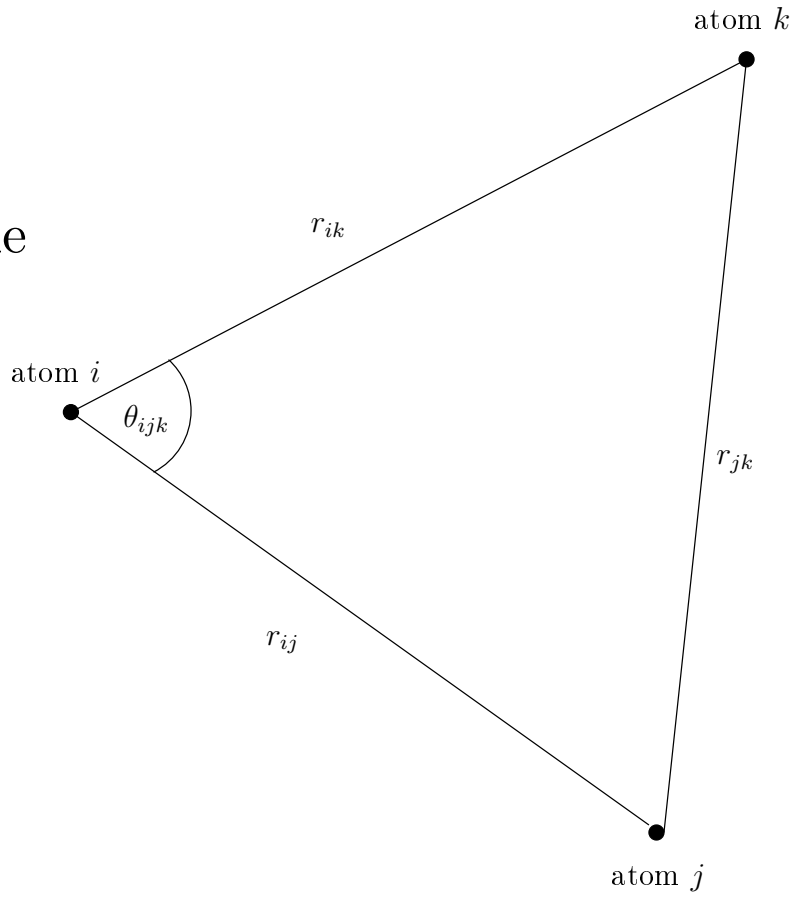
Experimentally observed:

- Minimal diameter of precipitation: 4 - 5 nm
- Equal orientation of Si and SiC (hkl)-planes

Simulation details

MD basics:

- Microscopic description of N particle system
- Analytical interaction potential
- Hamilton's equations of motion as propagation rule in 6N-dimensional phase space
- Observables obtained by time average



Application details:

- Integrator: Velocity Verlet, timestep: $1\,fs$
- Ensemble: NVT, Berendsen thermostat, $\tau = 100.0$
- Potential: Tersoff-like bond order potential

$$E = \frac{1}{2}\sum_{i \neq j} \mathcal{V}_{ij}, \quad \mathcal{V}_{ij} = f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right]$$

P. Erhart and K. Albe. Phys. Rev. B 71 (2005) 035211

Simulation details

Interstitial simulations:

- Initial configuration: $9 \times 9 \times 9$ unit cells Si
- Periodic boundary conditions
- $T = 0\,K$

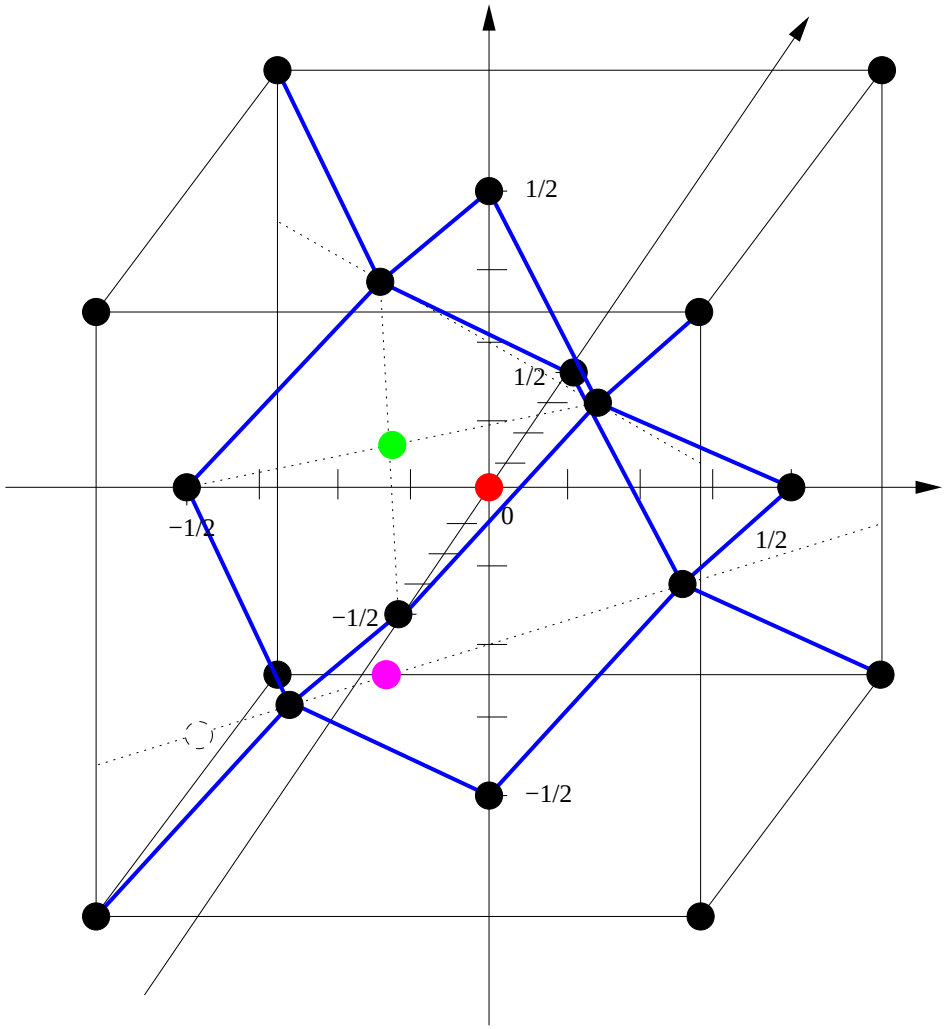
↓

Insertion of C / Si atom:

- $(0, 0, 0) \rightarrow$ tetrahedral
- $(-1/8, -1/8, 1/8) \rightarrow$ hexagonal
- $(-1/8, -1/8, -1/4)$, $(-1/4, -1/4, -1/4)$ $\rightarrow$ 110 dumbbell
- random positions (critical distance check)

↓

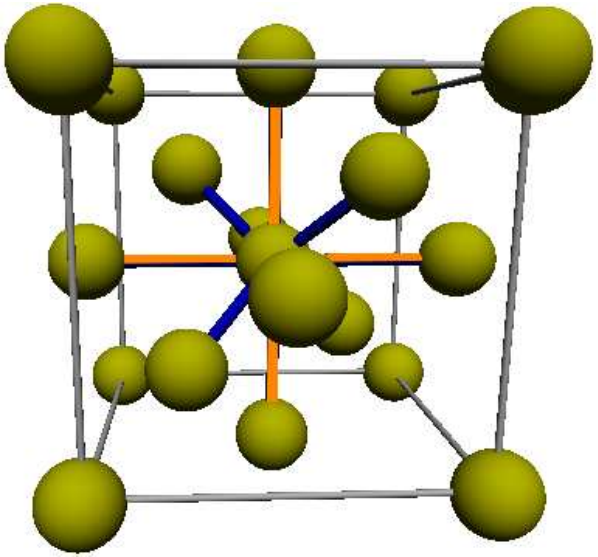
Relaxation time: $2\,ps$



Results - Si self-interstitial runs

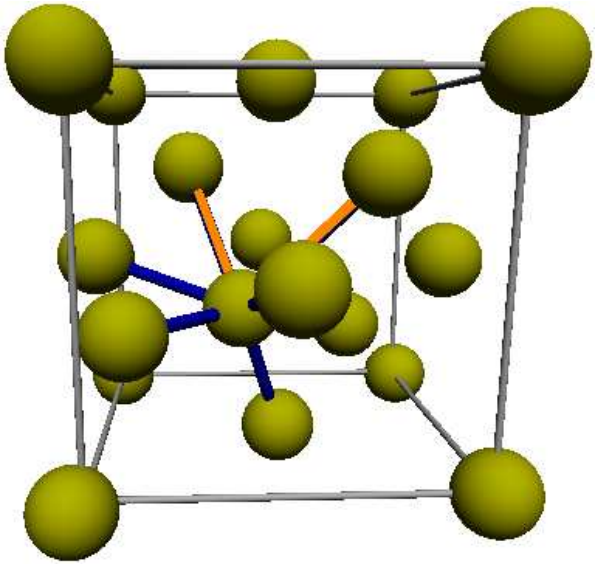
Tetrahedral

$E_f = 3.41\,eV$



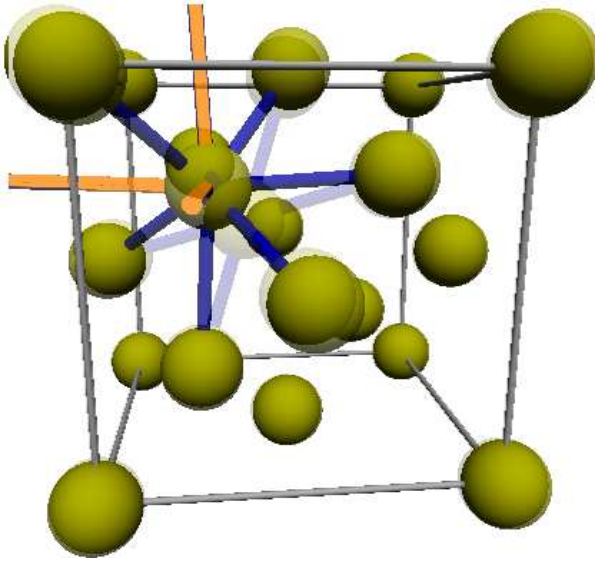
110 dumbbell

$E_f = 4.39\,eV$



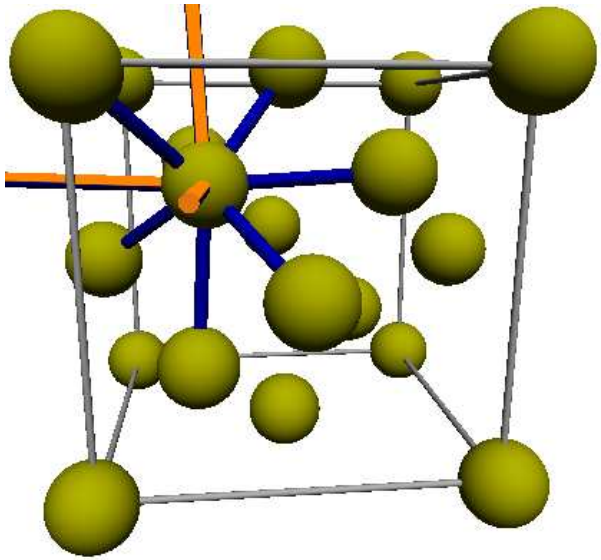
Hexagonal ▷

$E_f^\star \approx 4.48\,eV$ (unstable!)

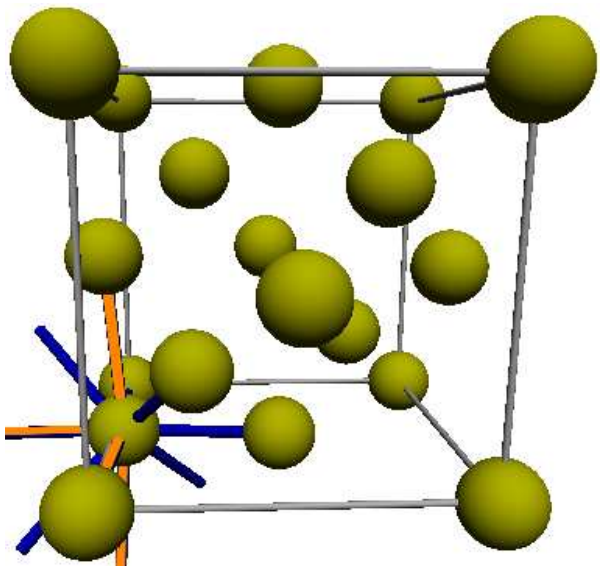


Random insertion

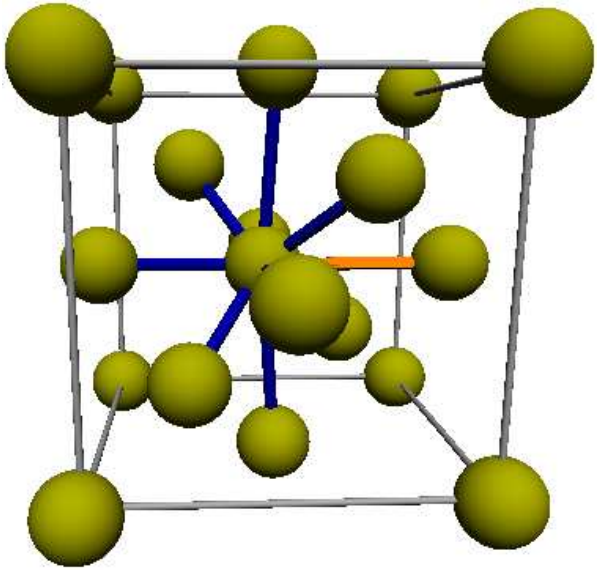
$E_f = 3.97\,eV$



$E_f = 3.75\,eV$



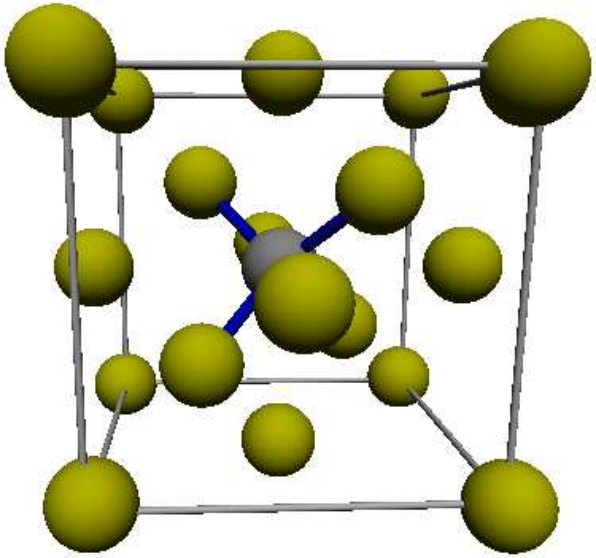
$E_f = 3.56\,eV$



Results - Carbon interstitial runs

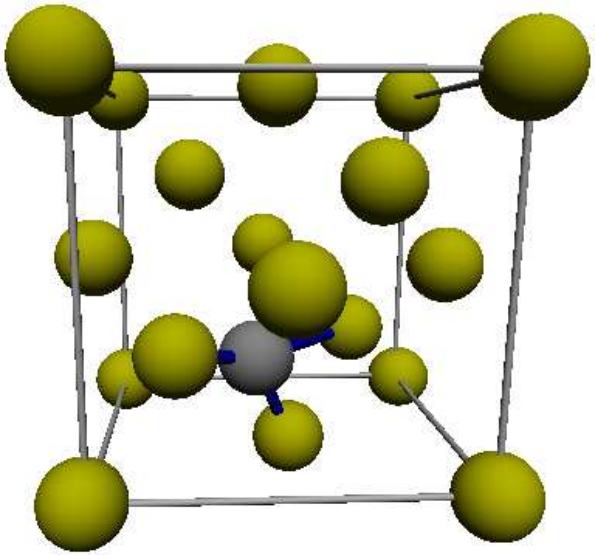
Tetrahedral

$E_f = 2.67\,eV$



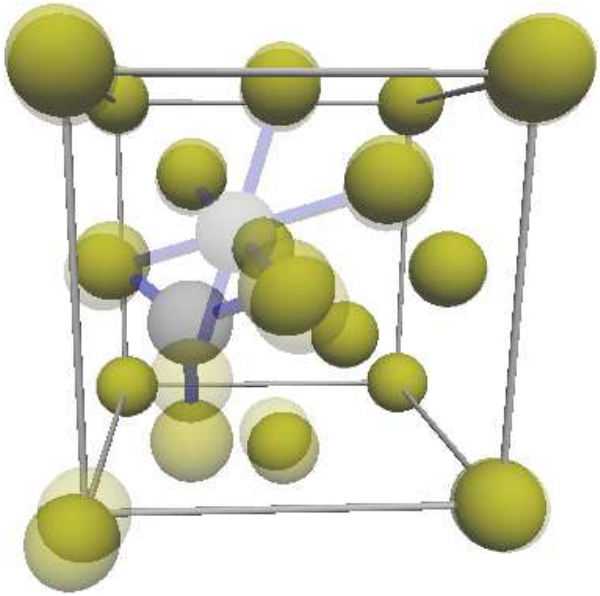
110 dumbbell

$E_f = 1.76\,eV$



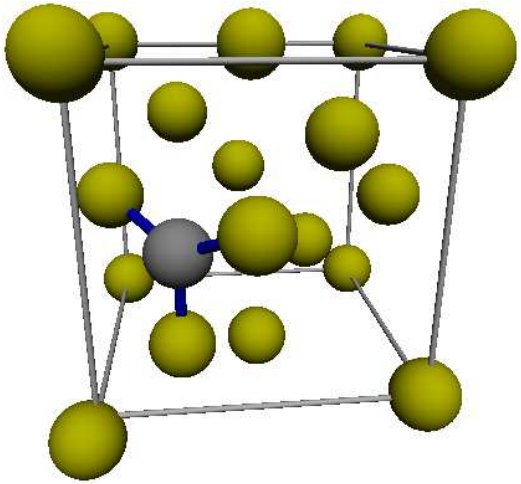
Hexagonal ▷

$E_f^\star \approx 5.6\,eV$ (unstable!)



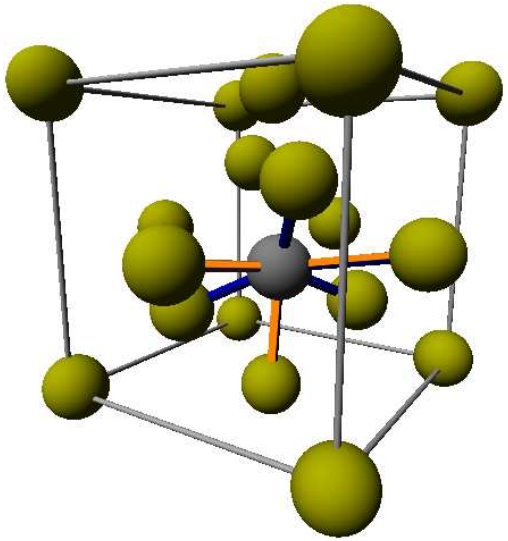
Random insertion

$E_f = 0.47\,eV$



001 dumbbell

$E_f = 1.62\,eV$



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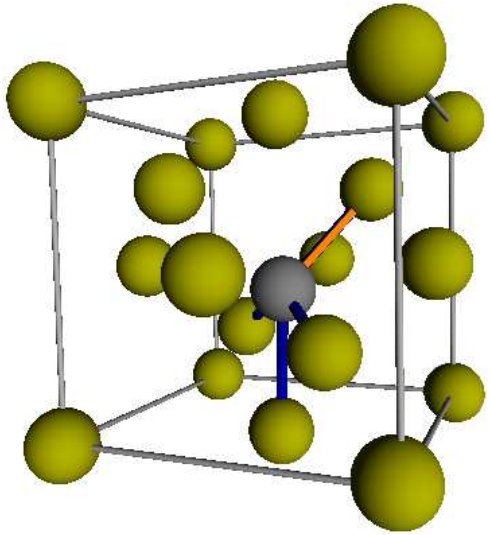

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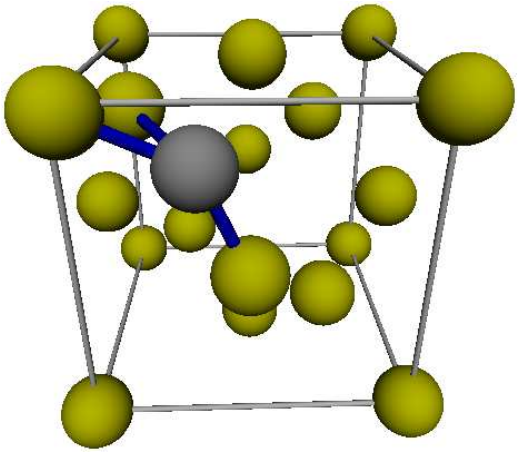


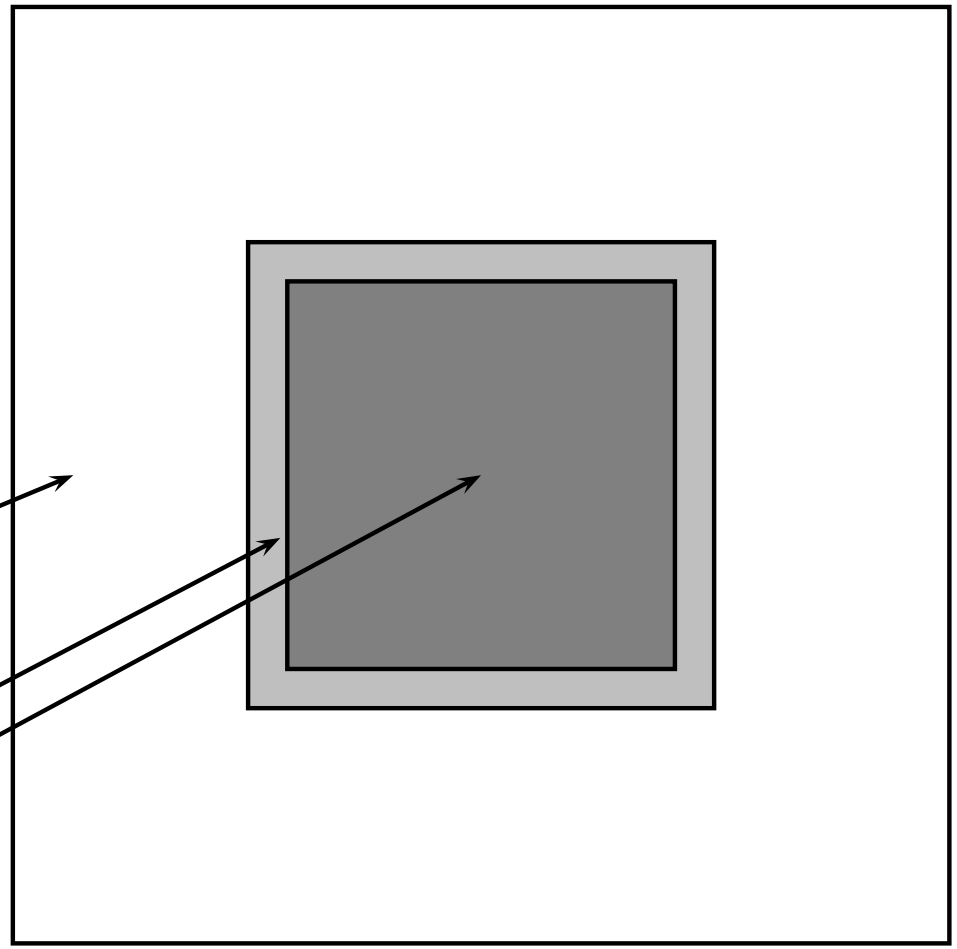
Simulation details

SiC precipitation simulations:

- Initial configuration: $31 \times 31 \times 31$ unit cells Si
- Periodic boundary conditions
- $T = 450\,^{\circ}C$
- Equilibration of E_{kin} and E_{pot} for 600 fs

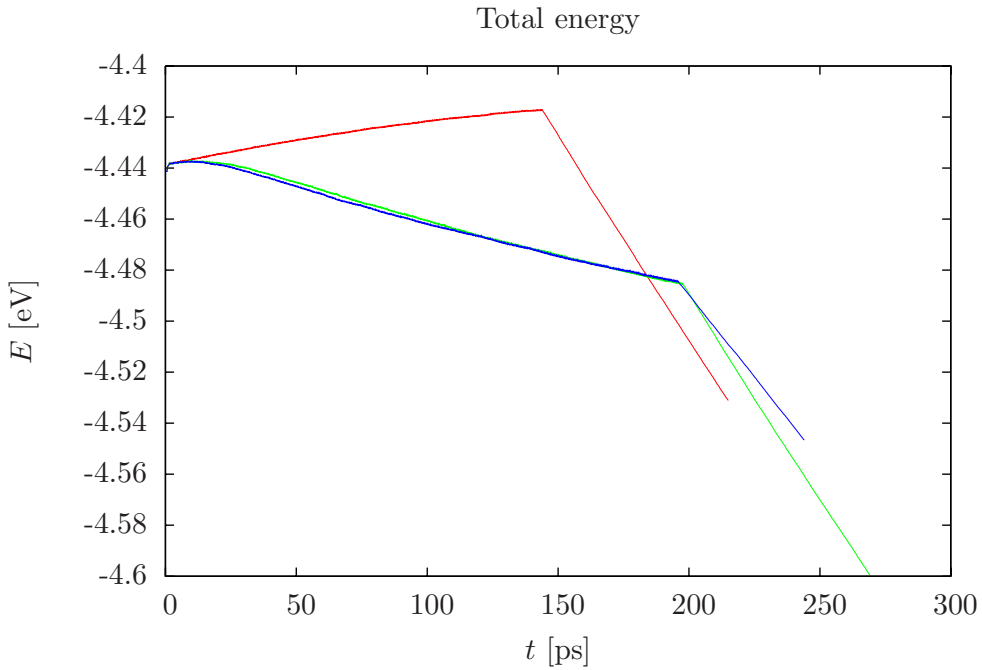
Insertion of 6000 carbon atoms at constant temperature into:

- Total simulation volume
- Volume of minimal SiC precipitation
- Volume of necessary amount of Si

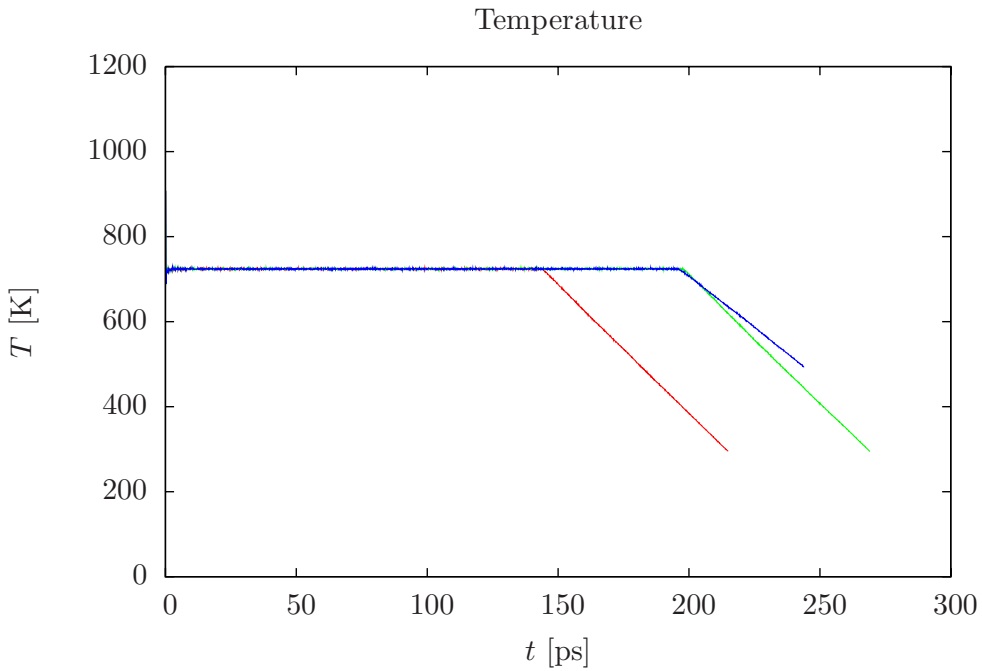


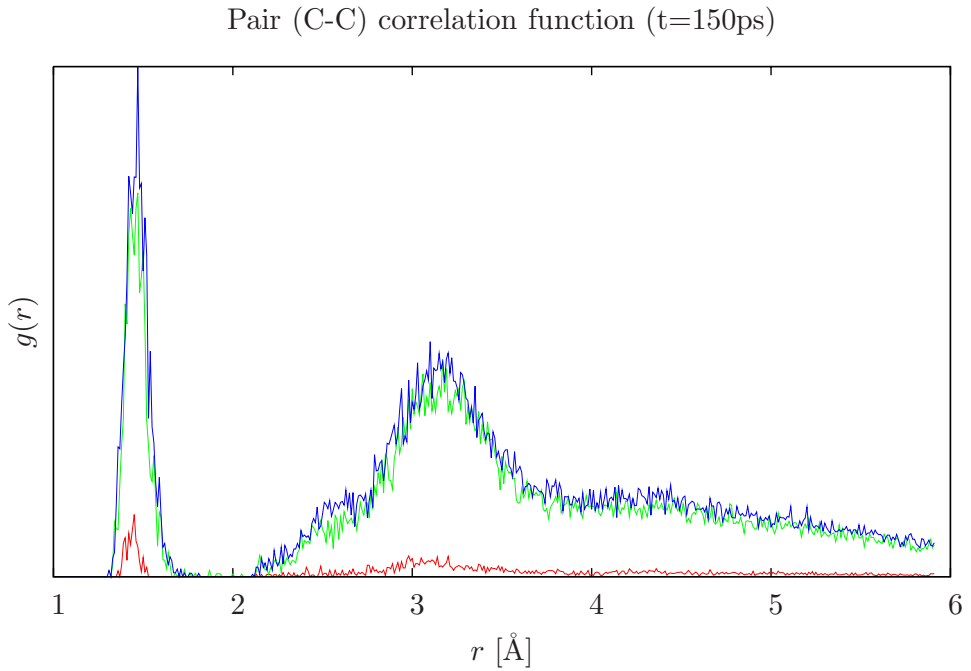
Cooling down to $20\,^{\circ}C$

Very first results of the SiC precipitation runs



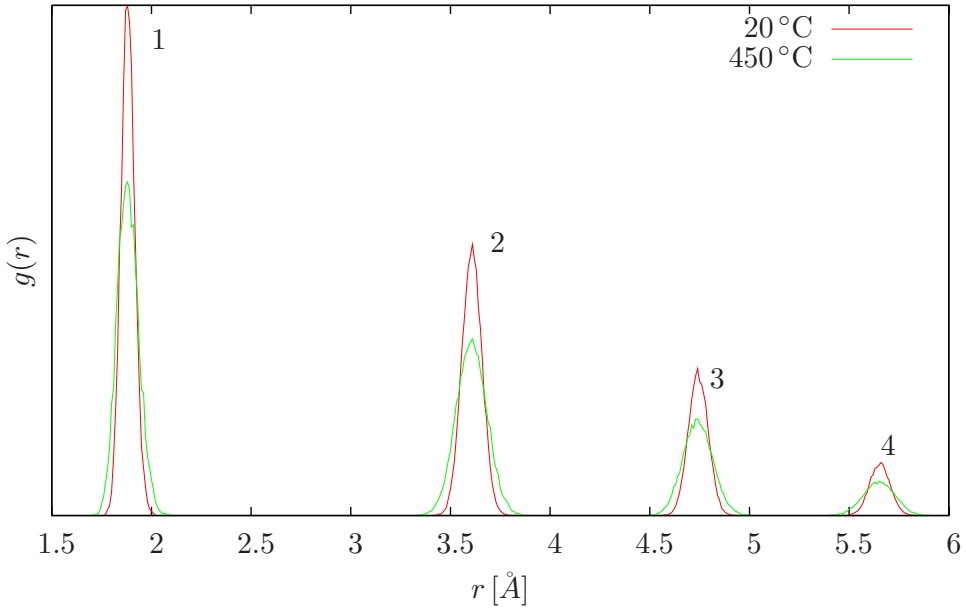
- Total simulation volume
- Volume of minimal SiC precipitation
- Volume of necessary amount of Si



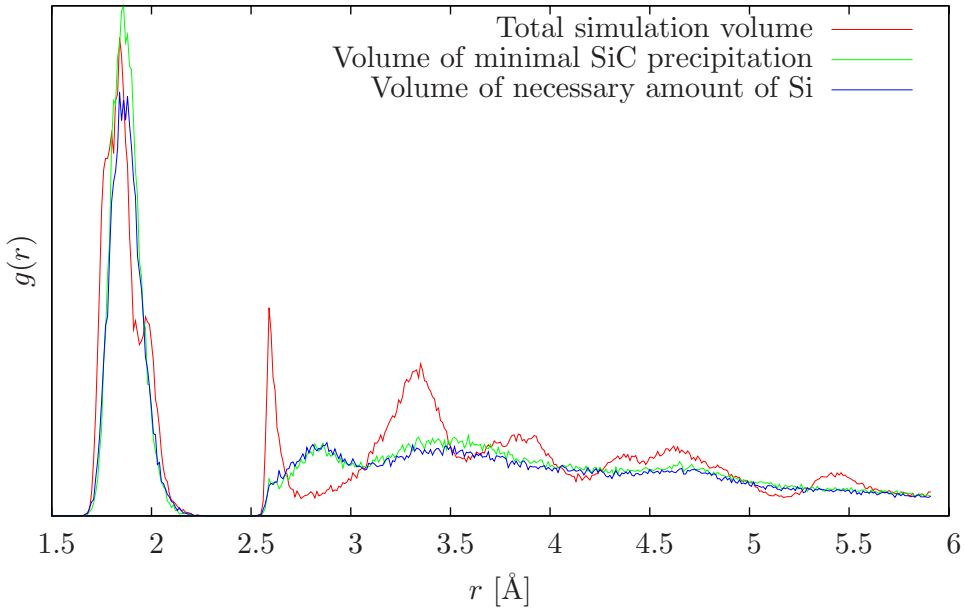


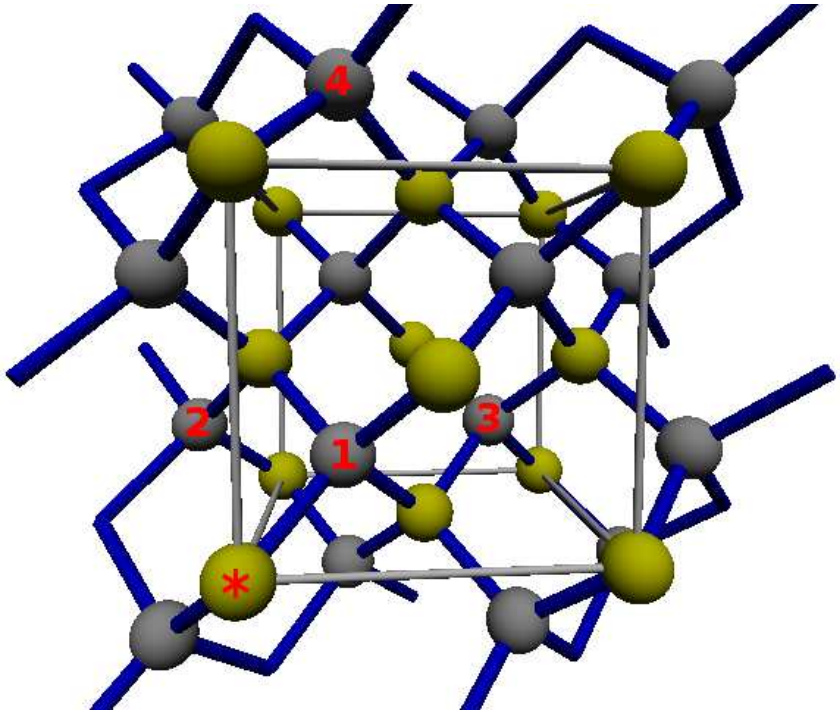
Very first results of the SiC precipitation runs

Reference pair (Si-C) correlation function of ideal 3C-SiC



Pair (Si-C) correlation function





Summary / Outlook

- Importance of understanding the SiC precipitation mechanism
- Interstitial configurations in silicon using the Albe potential
- Indication of SiC precipitation

- Displacement and stress calculations
- Refinement of simulation sequence to create 3C-SiC
- Analyzing self-designed Si/SiC interface