Molecular dynamics simulation of defect formation and precipitation in heavily carbon doped silicon

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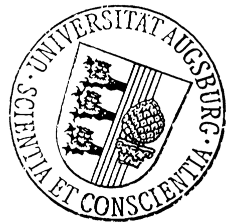
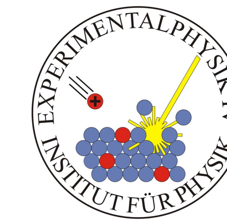


[1] Experimentalphysik IV, Institut für Physik, Universität Augsburg, Universitätsstr. 1, D-86135 Augsburg, Germany



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Motivation

Importance of the 3C-SiC precipitation process in silicon

- SiC is a promising wide band gap material for high-temperature, high-power, high-frequency semiconductor devices [1].
- 3C-SiC epitaxial thin film formation on Si requires detailed knowledge of SiC nucleation.
- Fabrication of high carbon doped, strained pseudomorphic $Si_{1-y}C_y$ layers requires suppression of 3C-SiC nucleation [2].

[1] J. H. Edgar, J. Mater. Res. 7 (1992) 235.
[2] J. W. Strane, S. R. Lee, H. J. Stein, S. T. Picraux, J. K. Watanabe, J. W. Mayer, J. Appl. Phys. 79 (1996) 637.

Crystalline silicon and cubic silicon carbide

Lattice types and unit cells:

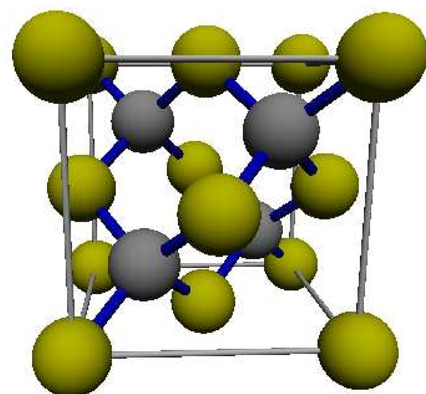
- Crystalline silicon (c-Si) has diamond structure
  ⇒ • and • are Si atoms
- Cubic silicon carbide (3C-SiC) has zincblende structure
  ⇒ • are Si atoms, • are C atoms

Lattice constants:

$$4a_{\text{c-Si}} \approx 5a_{\text{3C-SiC}}$$

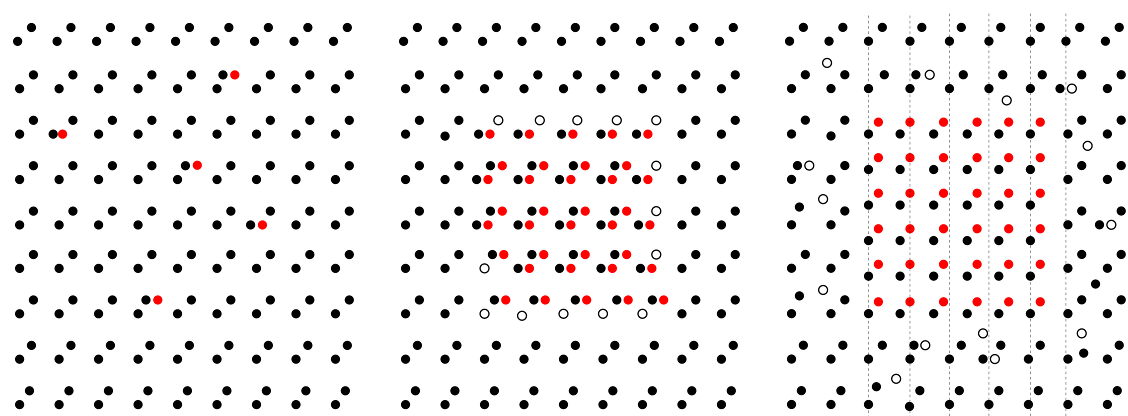
Silicon density:

$$\frac{n_{\text{3C-SiC}}}{n_{\text{c-Si}}} = 97,66\,\%$$



Supposed Si to 3C-SiC conversion

Schematic of the conversion mechanism



1. Formation of C-Si dumbbells on regular c-Si lattice sites
2. Agglomeration into large clusters (embryos)
3. Precipitation of 3C-SiC + Creation of interstitials

Experimental observations [3]

- Minimal radius of precipitates: 2 - 4 nm
- Equal orientation of c-Si and 3C-SiC (hkl)-planes

[3] J. K. N. Lindner, Appl. Phys. A 77 (2003) 27.

Simulation details

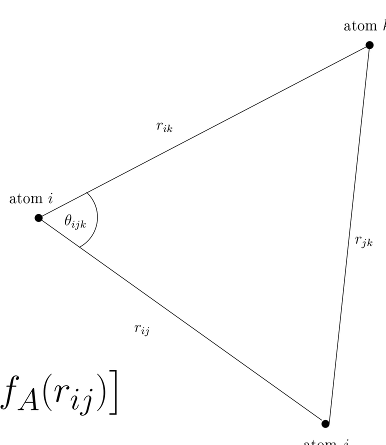
MD basics:

- Microscopic description of N particles
- Analytical interaction potential
- Propagation rule in 6N-dim. phase space: Hamilton's equations of motion
- Observables obtained by time or ensemble averages

Application details:

- Integrator: Velocity Verlet, timestep: 1 fs
- Ensemble: isothermal-isobaric NPT [4]
  - Berendsen thermostat: $\tau_T = 100$ fs
  - Brendsen barostat: $\tau_P = 100$ fs, $\beta^{-1} = 100$ GPa
- Potential: Tersoff-like bond order potential [5]

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



[4] L. Verlet, Phys. Rev. 159 (1967) 98.
[5] P. Erhart and K. Albe, Phys. Rev. B 71 (2005) 35211.

Interstitial configurations

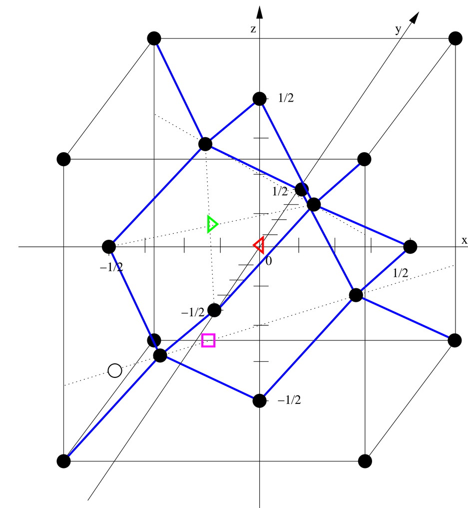
Simulation sequence:

- Initial configuration: 9 × 9 × 9 unit cells Si
- Periodic boundary conditions
- $T = 0$ K, $p = 0$ bar

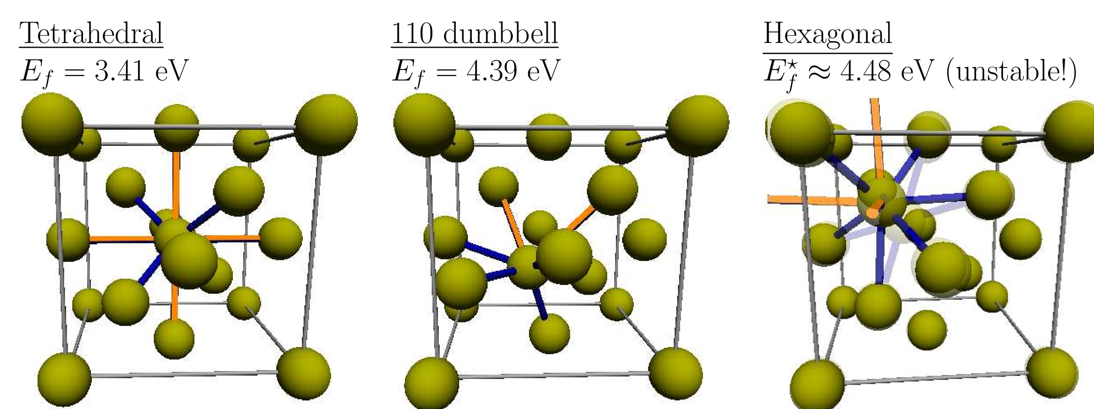
Insertion of C / Si atom:

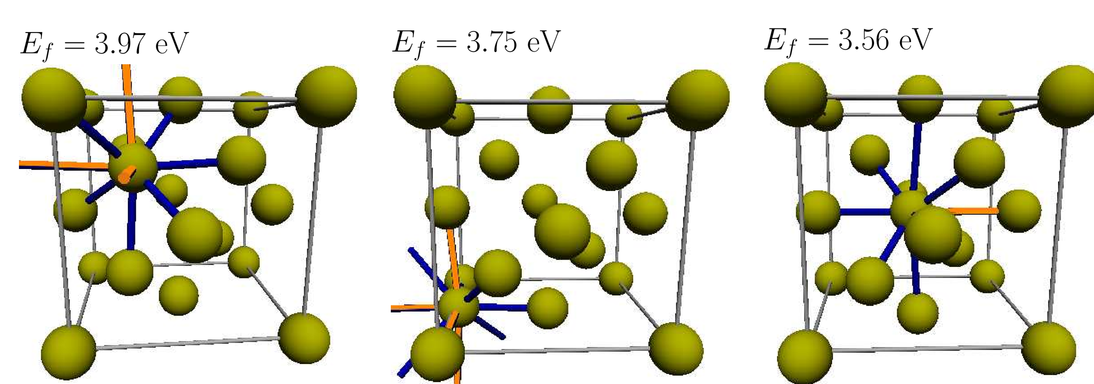
- $(0,0,0) \rightarrow$ tetrahedral (◁)
- $(-1/8,-1/8,1/8) \rightarrow$ hexagonal (▷)
- $(-1/8,-1/8,-1/4)$, $(-3/8,-3/8,-1/4)$ → 110 dumbbell (□,○)
- random positions (critical distance check)

Relaxation time: 2 ps

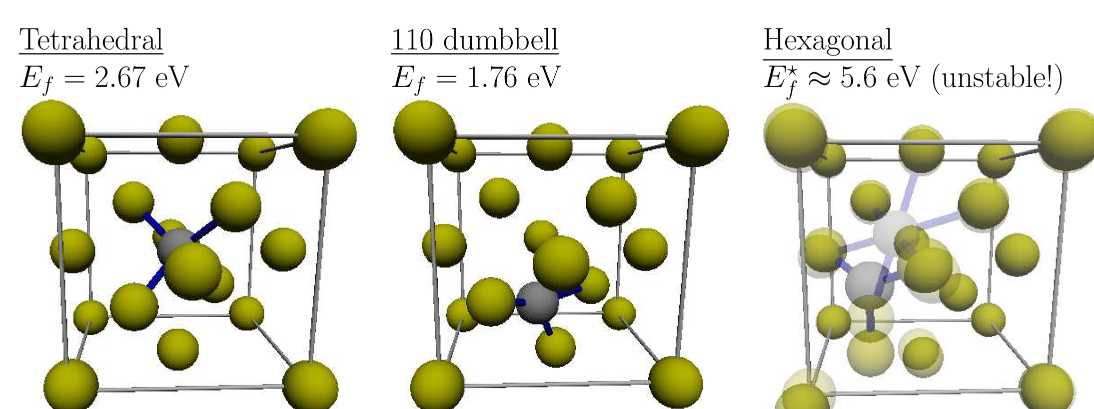


Si self-interstitial results:



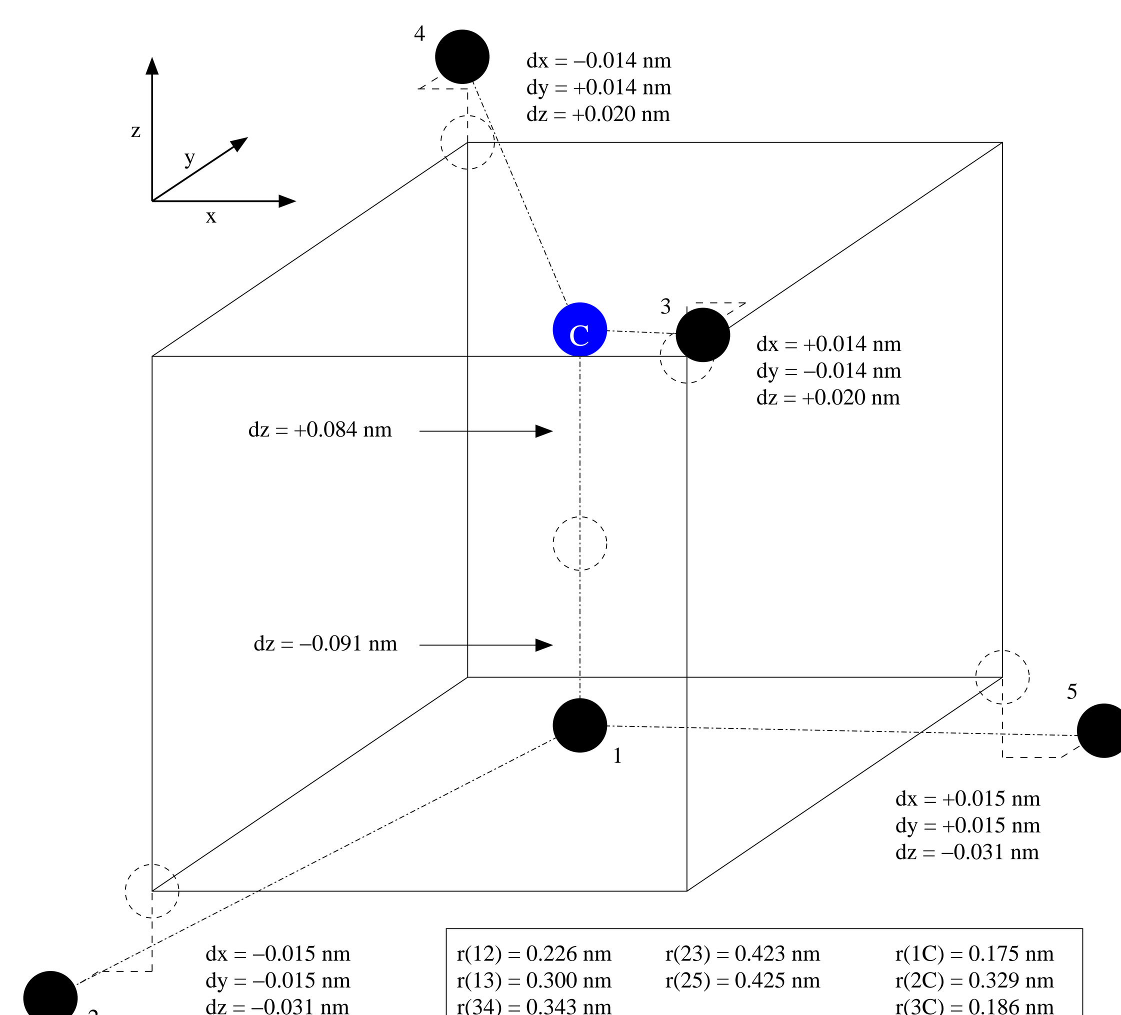


C in Si interstitial results:



<100> dumbbell configuration

- $E_f = 0.47$ eV
- Very often observed
- Most energetically favorable configuration
- Experimental evidence [6]



[6] G. D. Watkins and K. L. Brower, Phys. Rev. Lett. 36 (1976) 1329.

High C concentration simulations

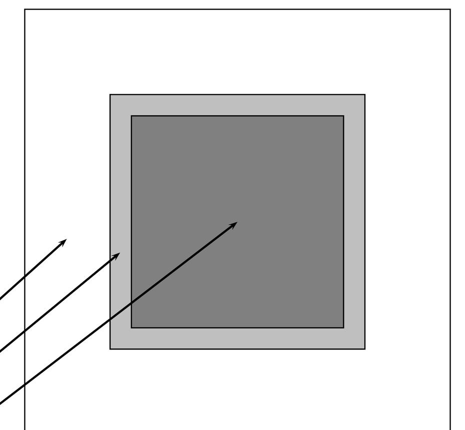
Simulation sequence:

- Initial configuration: 31 × 31 × 31 unit cells Si
- Periodic boundary conditions
- $T = 450\,°$C, $p = 0$ bar
- Equilibration of E_{kin} and E_{pot}

Insertion of 6000 carbon atoms at constant temperature into V_1 or V_2 or V_3:

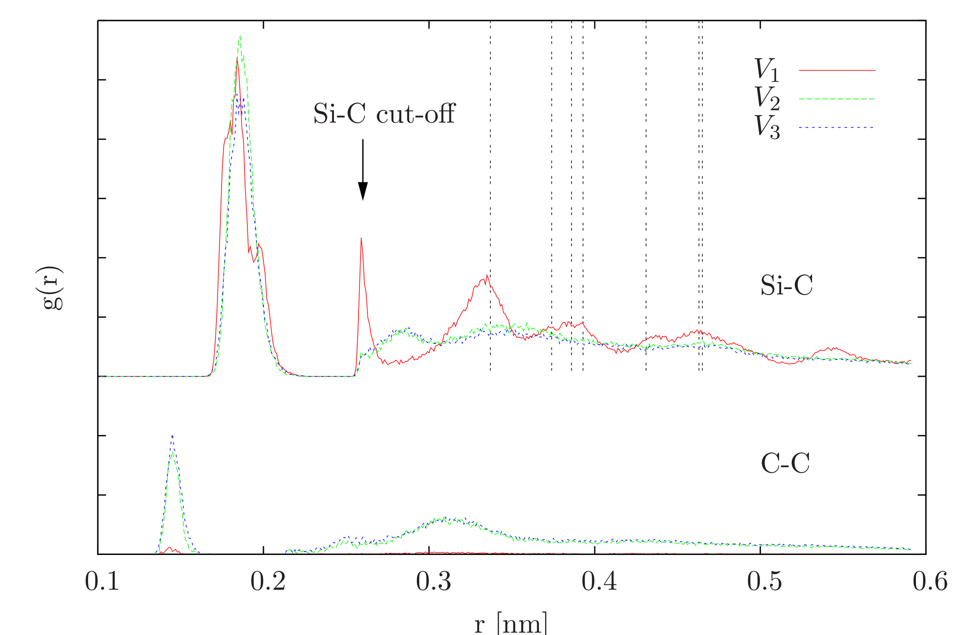
- Total simulation volume V_1
- Volume of minimal 3C-SiC precipitation V_2
- Volume of necessary amount of Si V_3

Cooling down to 20 °C



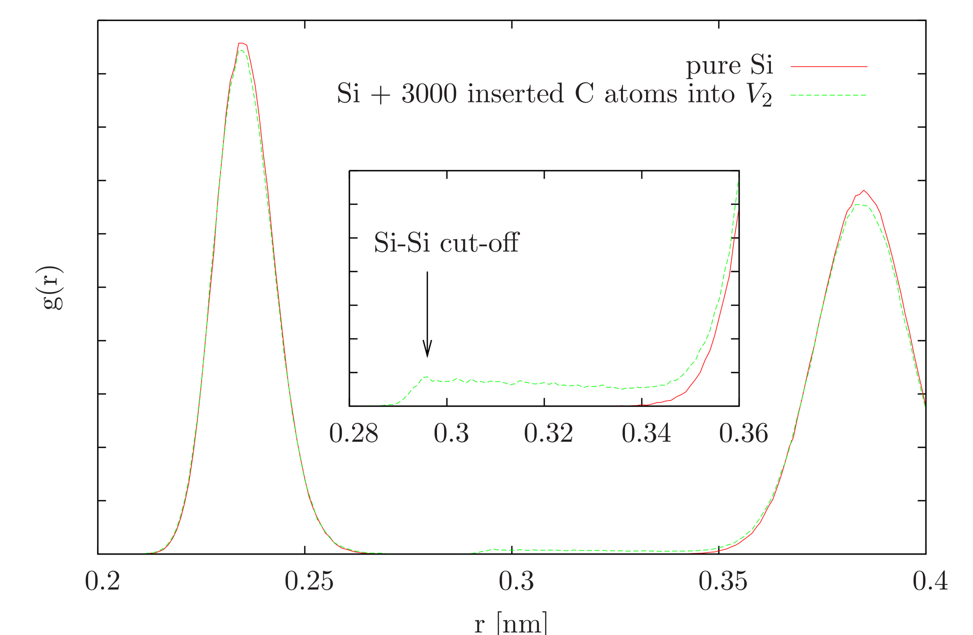
Results:

Si-C and C-C pair correlation function:



Dashed vertical lines: Further calculated C-Si distances in the <100> C-Si dumbbell interstitial configuration

Si-Si pair correlation function:



Interpretation:

- C-C peak at 0.15 nm similar to next neighbour distance of graphite or diamond
  ⇒ Formation of strong C-C bonds (almost only for high C concentrations)
- Si-C peak at 0.19 nm similar to next neighbour distance in 3C-SiC
- C-C peak at 0.31 nm equals C-C distance in 3C-SiC
  (due to concatenated, differently oriented <100> dumbbell interstitials)
- Si-Si shows non-zero g(r) values around 0.31 nm like in 3C-SiC
  and a decrease at regular distances
  (no clear peak, interval of enhanced g(r) corresponds to C-C peak width)
- Low C concentration (i.e. V_1): The <100> dumbbell configuration
  - is identified to stretch the Si-Si next neighbour distance to 0.3 nm
  - is identified to contribute to the Si-C peak at 0.19 nm
  - explains further C-Si peaks (dashed vertical lines)

  ⇒ C atoms are first elements arranged at distances expected for 3C-SiC
  ⇒ C atoms pull the Si atoms into the right configuration at a later stage
- High C concentration (i.e. V_2 and V_3):
  - High amount of damage introduced into the system
  - Short range order observed but almost no long range order

  ⇒ Start of amorphous SiC-like phase formation
  ⇒ Higher temperatures required for proper SiC formation

Conclusion

- <100> C-Si dumbbell interstitial configuration is observed to be the energetically most favorable configuration
- For low C concentrations C atoms introduced as differently oriented C-Si dumbbells in c-Si are properly arranged for 3C-SiC formation
- For high C concentrations an amorphous SiC-like phase is observed which suggests higher temperature simulation runs for proper 3C-SiC formation

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