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Molecular Dynamics Simulations of the Sputtering of β-SiC by Ar

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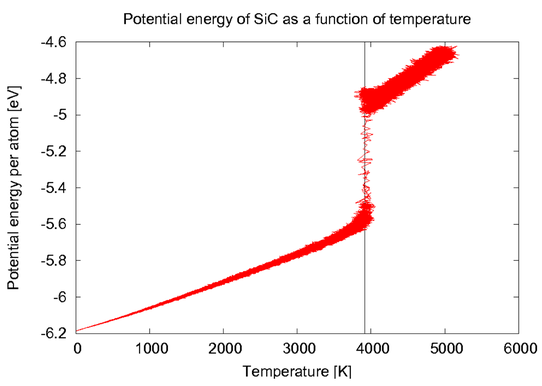
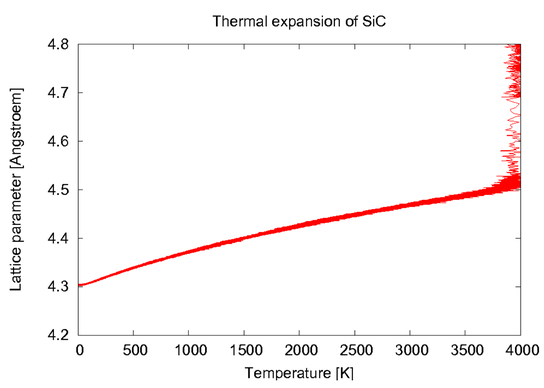
Introduction

- The overall research goal is to use molecular dynamics simulations in combination with experimental validation for the development of improved SiC and SiN single- and bilayer coatings, and multilayer SiC/SiN nanolaminates, which are deposited by magnetron sputtering onto silicon and/or steel. These materials are characterised by a high oxidation, wear and thermal resistance.
- As a first step for the development of SiC/SiN nanolaminates the sputtering of a SiC-target at 700 K by argon was simulated by the method of molecular dynamics using the Tersoff potential for the Si-C interaction and tabulated ZBL pair potential for the interaction with argon.

Thermal expansion and melting temperature of SiC

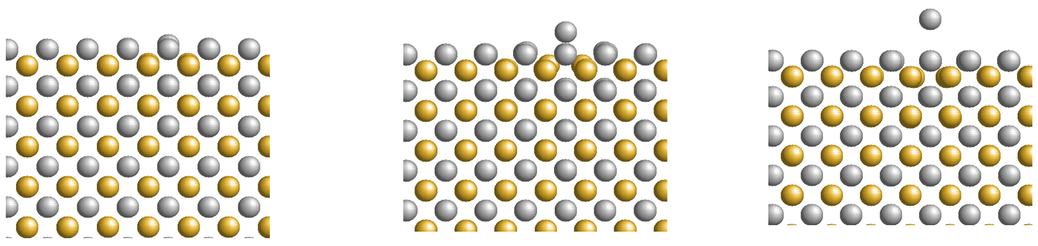
- Cubic SiC-target consisting of 4096 atoms heated from 0K to 5000K
- Npt-ensemble with external pressure (isotropic volume scaling) and temperature (Nose-Hoover thermostat) control
- Imposed temperature linearly varied over 10^8 time steps, each time step being 0.1 fs long
- Discontinuity in the temperature regime indicates phase transition
- Coefficient of thermal expansion of β-SiC is $\alpha=1.1\cdot10^{-5}$ and the melting temperature is 3920 K

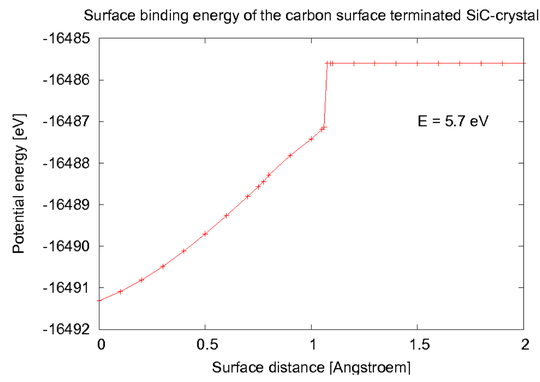


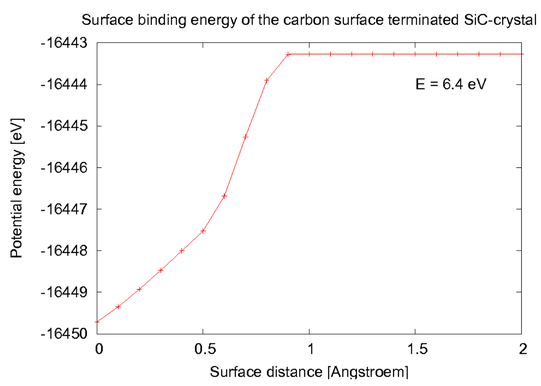


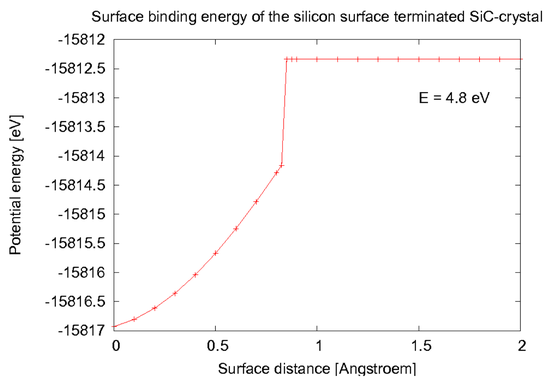
Surface binding energy

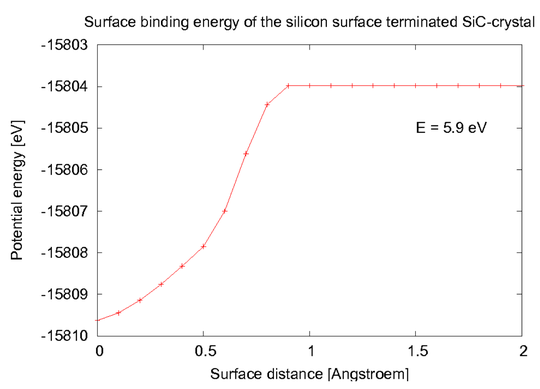
- For sputtering, the kinetic energy of the surface atoms must exceed the surface binding energy.
- Distinction between four surface binding energies, two types of surfaces, with and without surface recombination





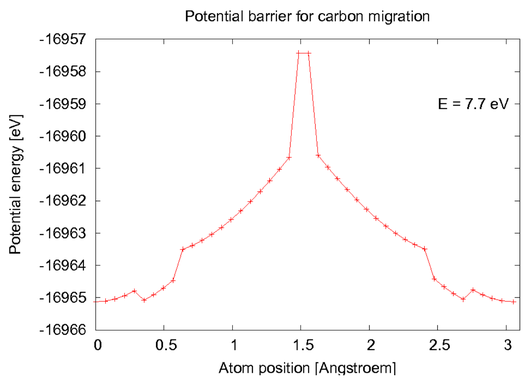


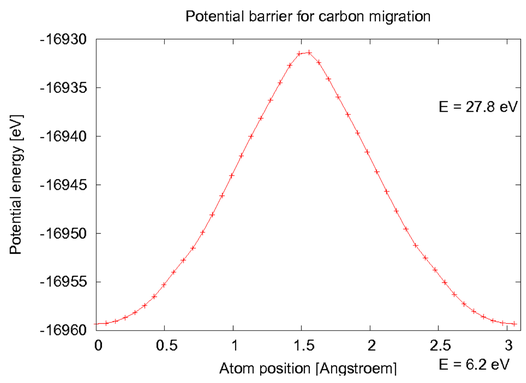


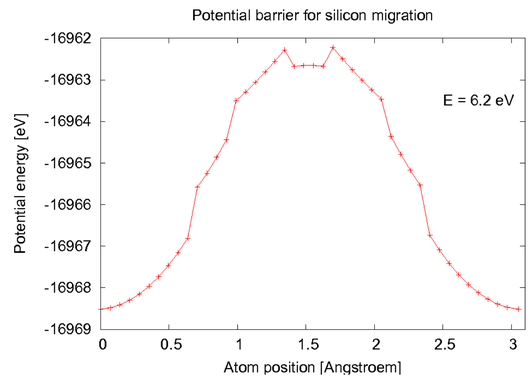


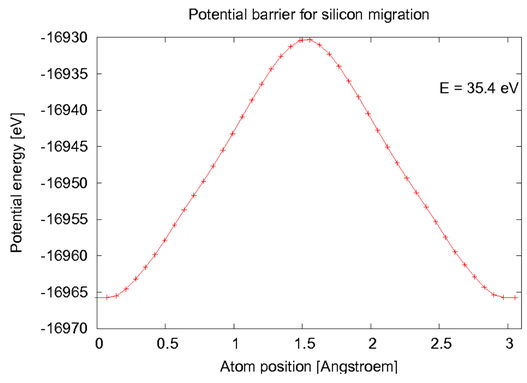
Migration energy

- Mobility of atoms and holes inside an SiC-crystal
- Distinction between two sublattices (Si and C)
- Potential barriers of different heights depending on the considered sublattice and the behaviour of surrounding atoms



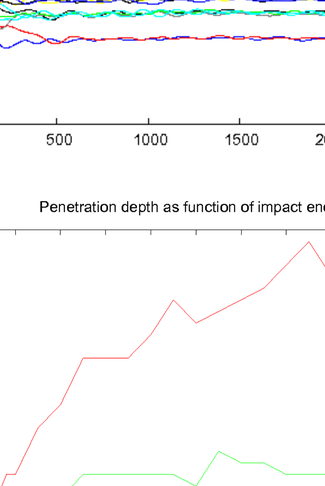




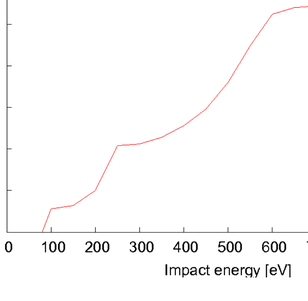


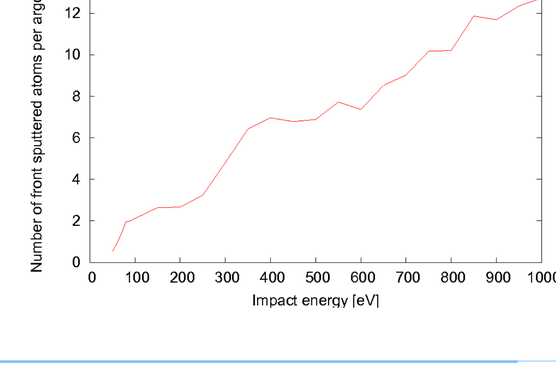
Sputtering of beta-SiC by Ar

- Monocrystal of β-SiC in the dimensions of 10·10·20 unit cells
- Equilibriation of the target material at 700K using npt-simulation as described. Usage of 50 thermic equivalent probes to achieve statistics



- Impact energies of the argon ion between 50 eV and 1 keV
- Distinction between C-surface and Si-surface terminated single crystal





- Analysis of different data types, in particular the penetration depth, front- and back sputtered atoms (sputter yield)
- Automatisation due to large amount of data

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