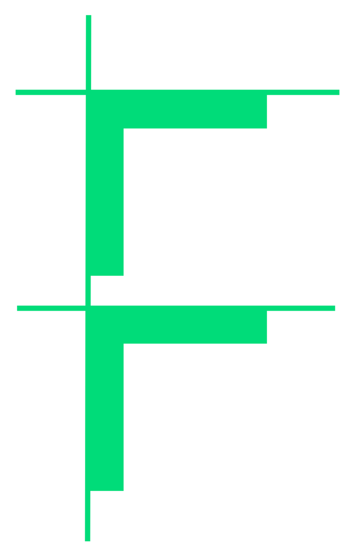

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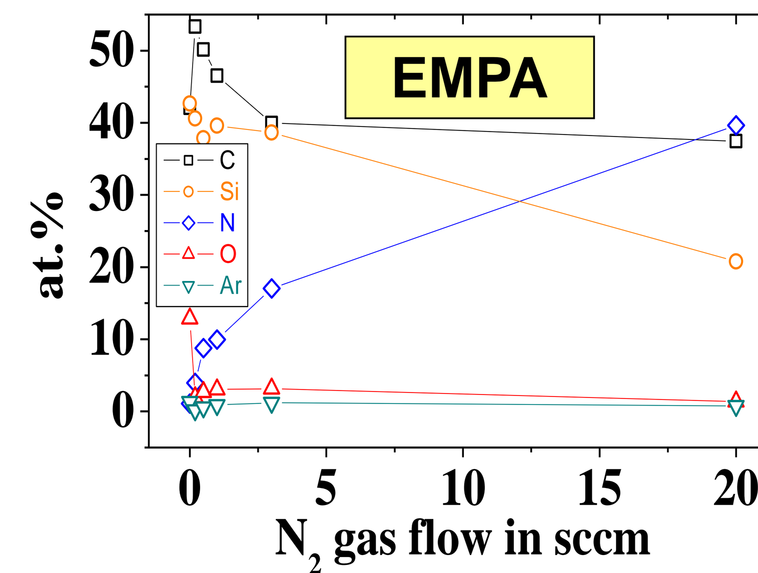
Sputter deposition of single layer Si-C-N films: molecular dynamics simulation and experimental validation of structure-property-correlations

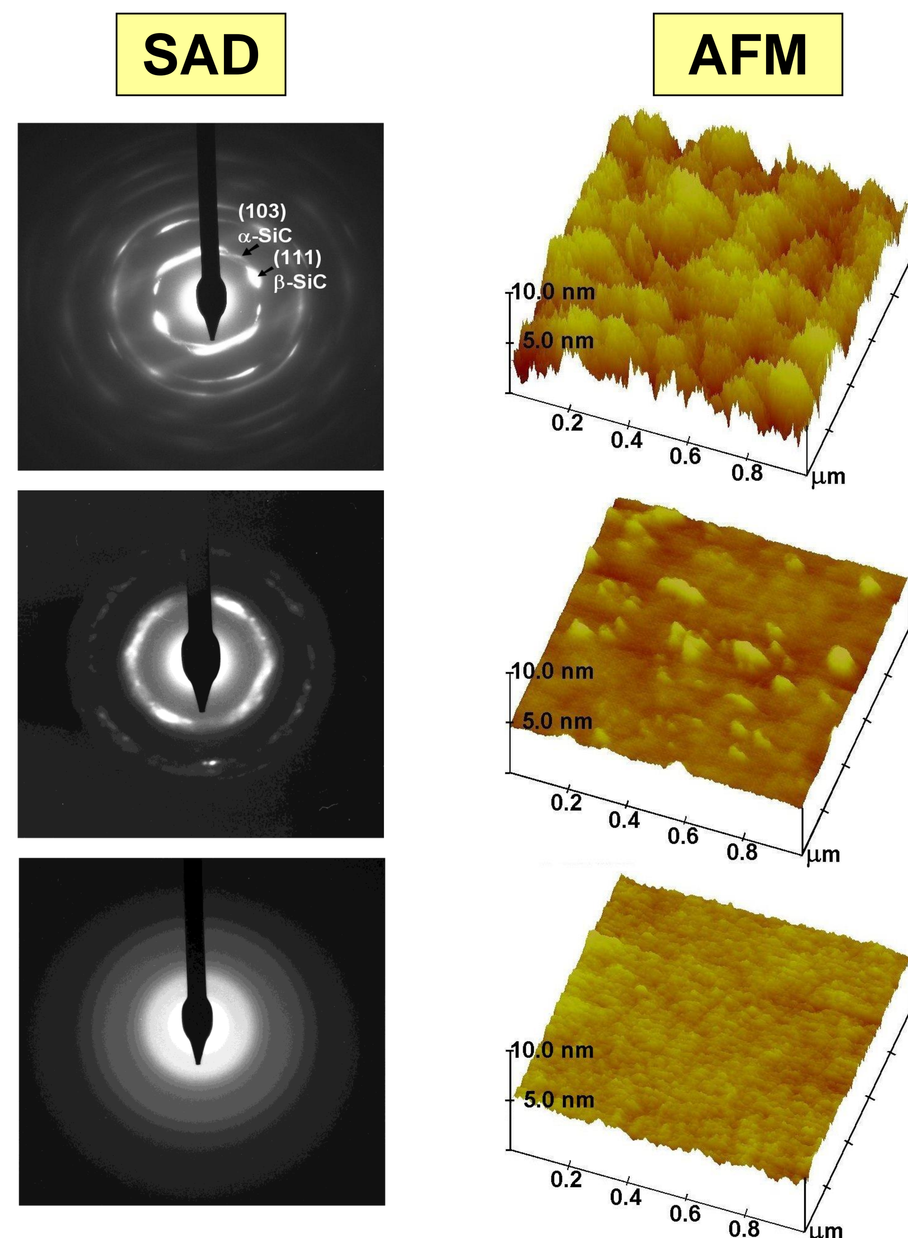
Experimental results

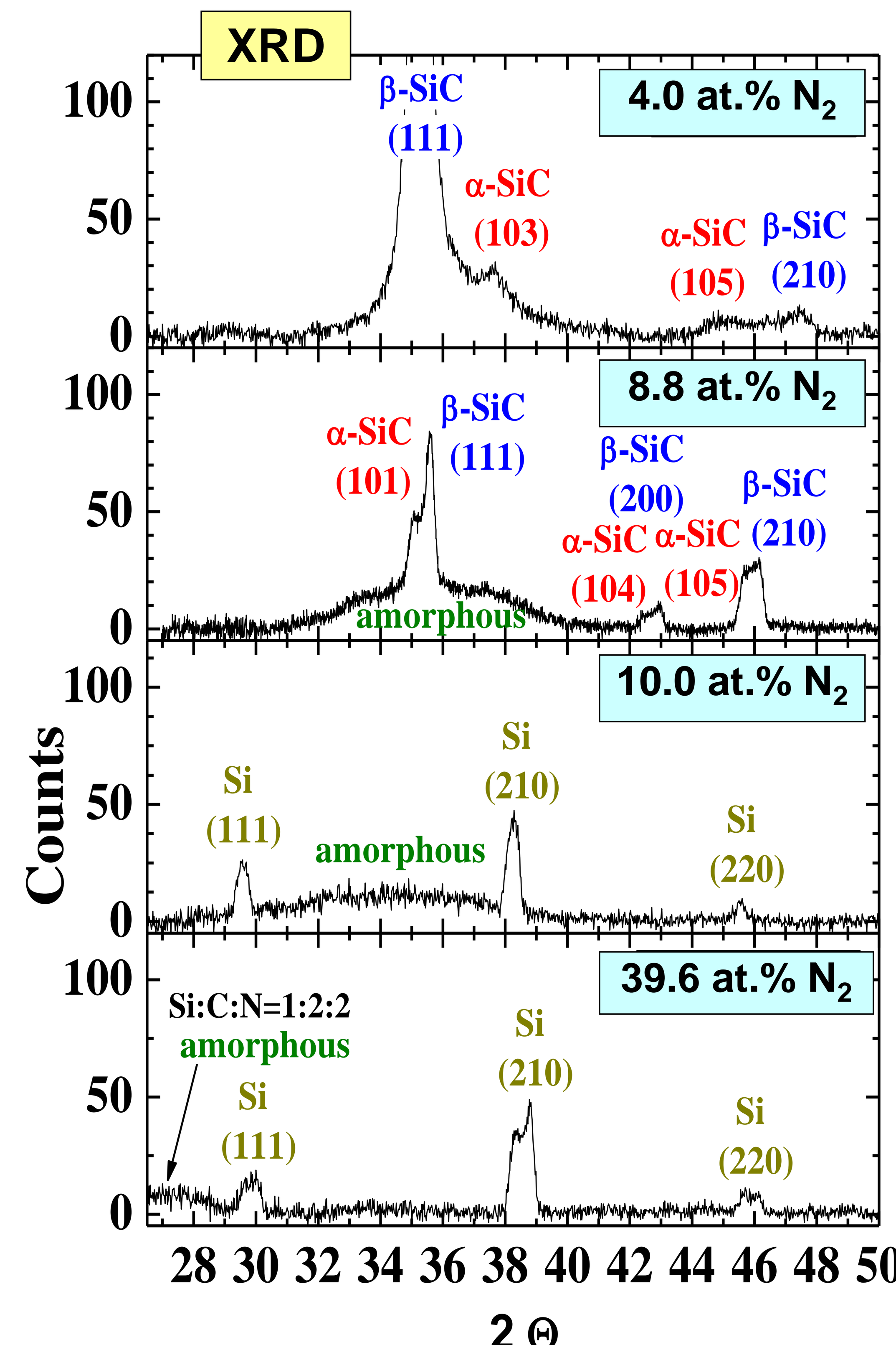
Preparation and Composition

- RF magnetron sputtering from a SiC target in an Ar/N_2 atmosphere (T_s = 800 °C, U_s = 0 V) on Si and hard metal substrates with N_2 gas flow variation (0-20 sccm)
- Correlation of constitution, microstructure and properties

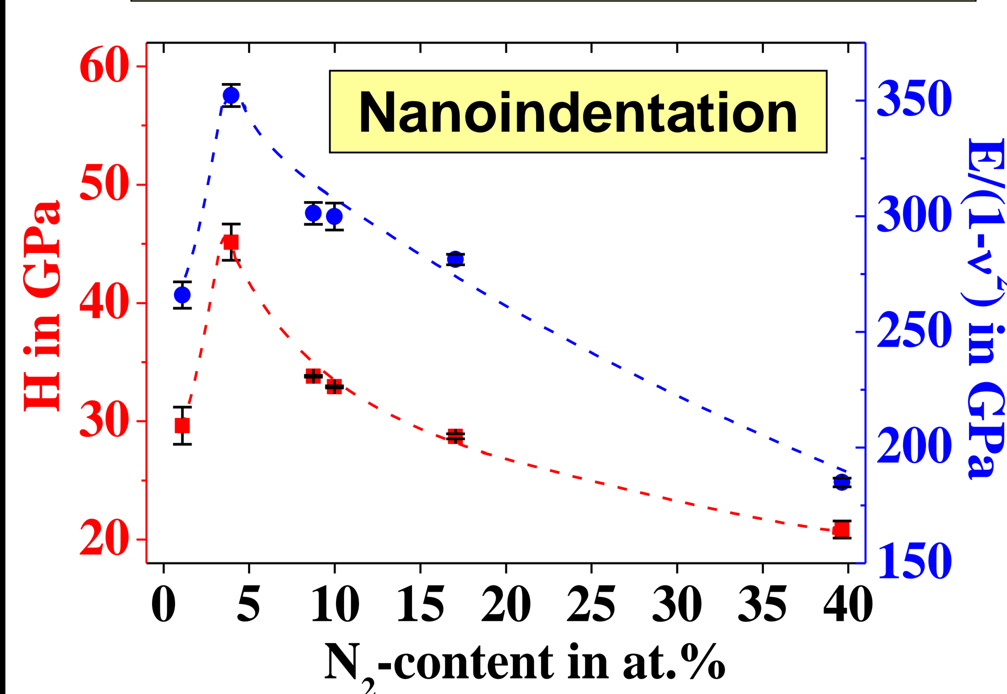


Microstructure and surface topography





Mechanical properties



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Molecular dynamics simulations

Sputtering

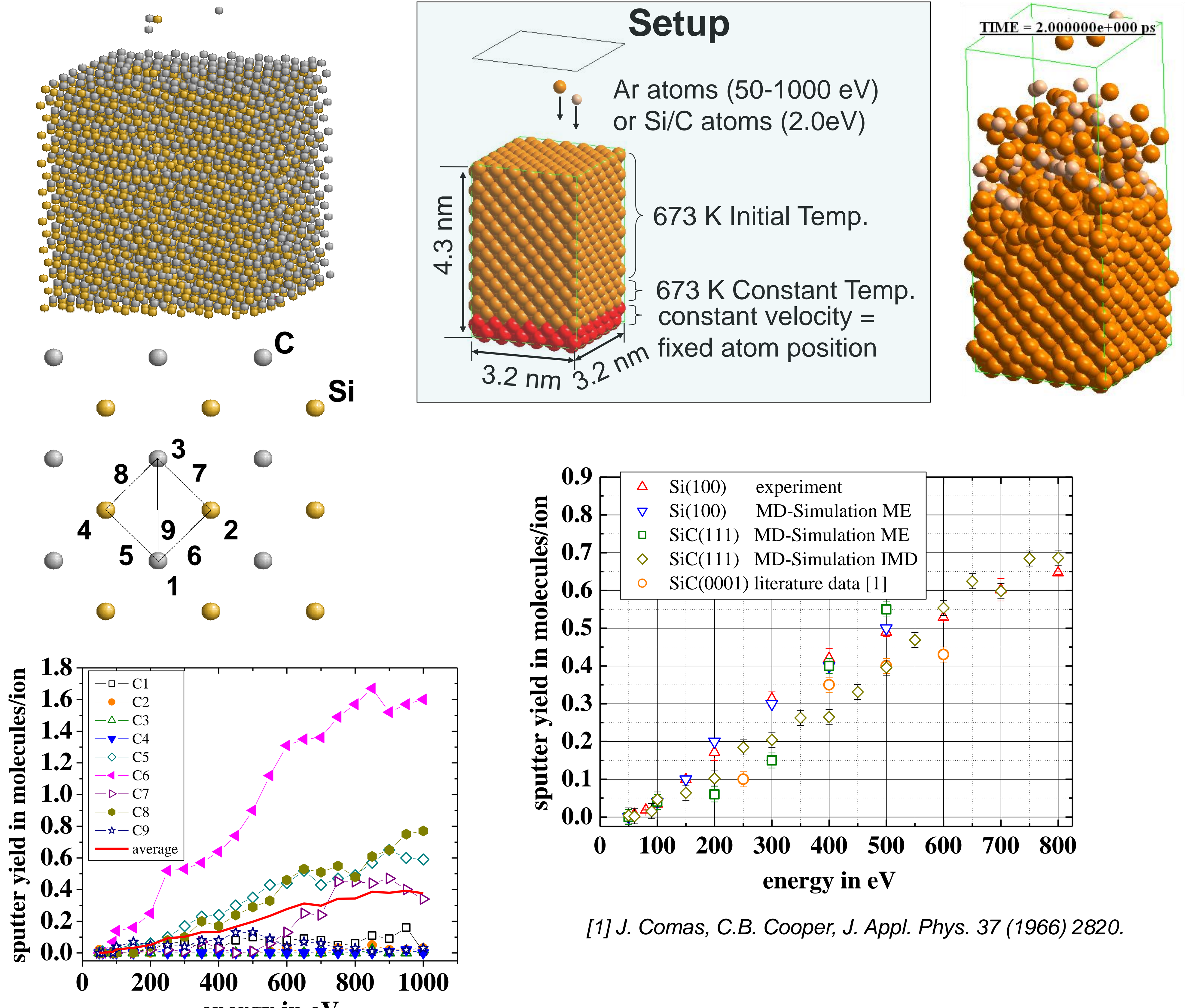
Target: C-terminated SiC, T_S = 673 K, potential: Tersoff
x,y-axis: periodic boundary condition
z-axis: open surface
- 3072 Si atoms, 3072 C atoms (ME software)
- 8000 Si atoms, 8000 C atoms (IMD software)

Ar: energy: 50-1000 eV, potential: ZBL, angle: 180°
- 1 Ar at random every 24 ps, ensemble: NTV, Nosé thermostat (ME)
- equilibriation at 673K using NPT-simulation 1 Ar on 9 coordinates for 50 thermically equivalent samples using NVE ensemble (IMD)

Deposition

Substrate: 2592 Si atoms, T_S = 673 K, potential: Tersoff
x,y-axis: periodic boundary condition
z-axis: open surface (ME)

Si/C: 1 Si/C atom every 1.25 ps, incidence angle: 180°, energy: 2 eV
Number of deposited atoms: 800
MD step: 1 fs, ensemble: NTV (ME)



[1] J. Comas, C.B. Cooper, J. Appl. Phys. 37 (1966) 2820.

Conclusions

As the first experimental step thin Si-C-N films have been deposited with systematic variation of the N_2 flow rate and its influence on the constitution, the microstructure and the mechanical properties was investigated. At a low N_2 content of 4.0 at.% in the film, a two-phase microstructure with nanocrystalline grains of 5-10 nm is formed with a hardness value of 45 GPa is formed.

As the first simulation step the sputtering of a SiC-target at 673 K by argon was simulated using the Tersoff potential for the Si-C interaction and ZBL pair potential for the interaction with argon and the sputter yield and the and the ranges of Ar ions and sputtered Si and C atoms were determined as a function of the energy of the incident Ar atoms.

HELMHOLTZ GEMEINSCHAFT

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