Molecular dynamics study on defect formation in SiC film

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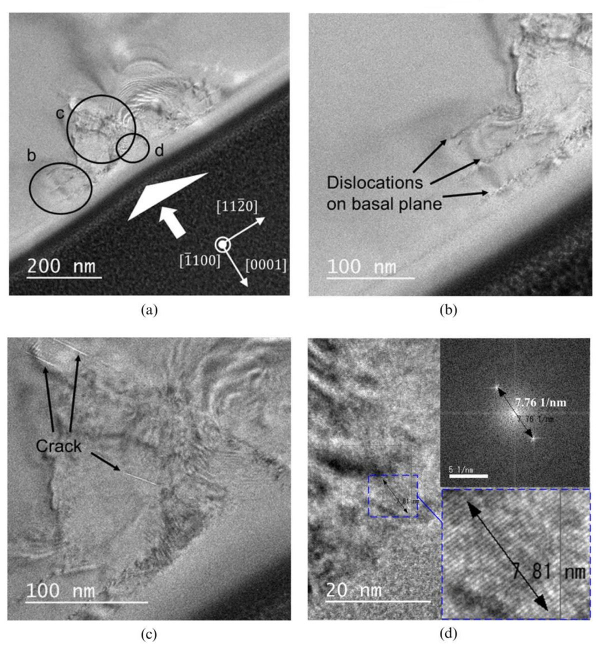
Highlights

- Our molecular dynamics simulations have revealed the dependence of temperature and crystallographic orientation on defect formation in single crystalline SiC.
- High temperature causes the transition of formed defects from perfect dislocations to partial dislocations with stacking faults.
- Impressions after nanoindentation exhibit obvious crystal anisotropy on its symmetry and pileup patterns.

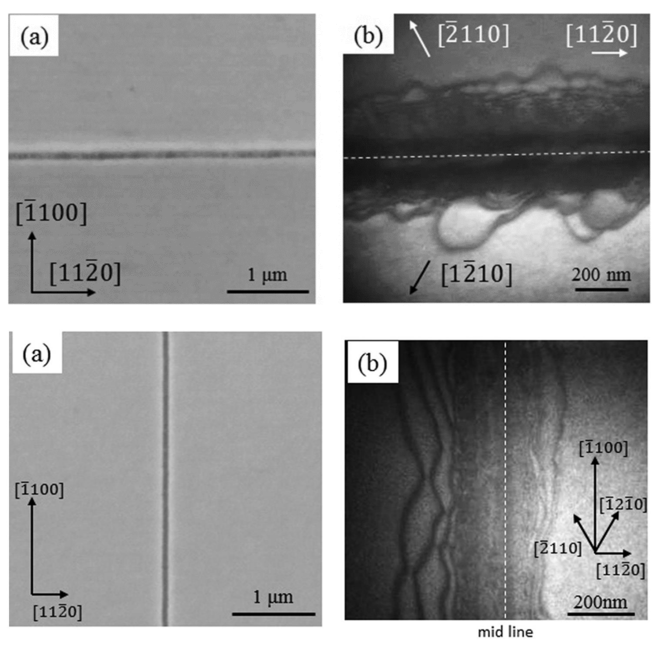
Introduction

Silicon carbide (SiC) is a promising candidate as a semiconductor for next-generation power electronics devices. Despite numerous experimental studies, it is still a great challenge to understand mechanical properties and defect formation process at an atomistic level.
Objectives: To clarify plastic deformation mechanism and defect formation criteria in SiC.

Nanoindentation[1]



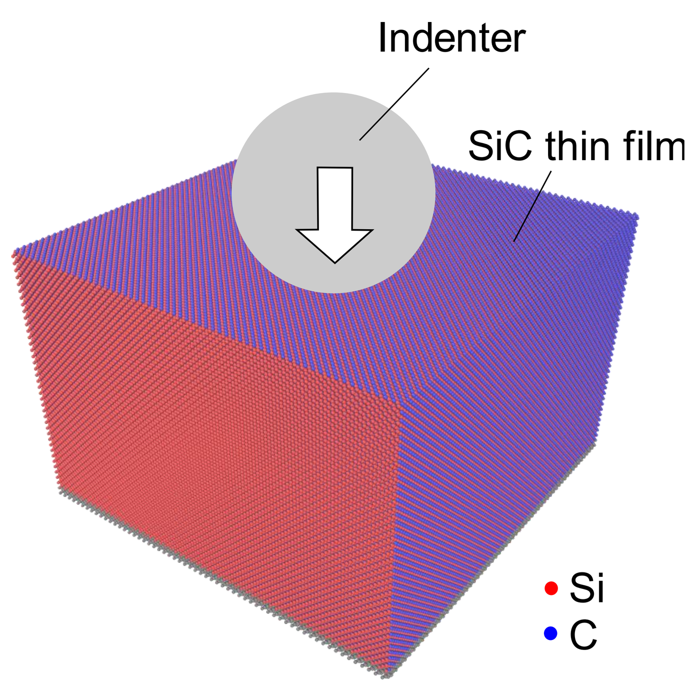
Nanoscratch[2]



[1]Matsumoto *et al.*, J.Phys. D: Appl. Phys. **50**, 265303 (2017).
[2]Sako *et al.*, J. Appl. Phys. **119**, 135702 (2016).

Method

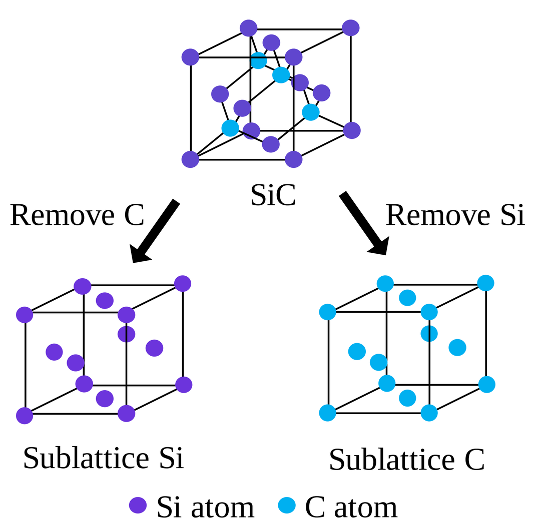
Nanoindentation



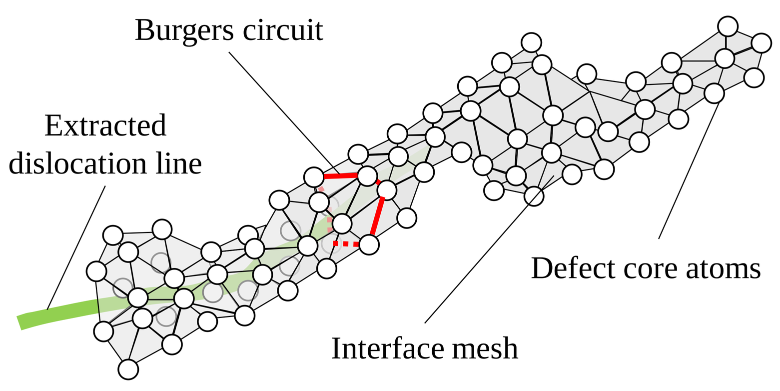
Simulation conditions

Property	Value
Temperature [K]	300, 1000 1500, 2000
Number of atom	1150000
Indenter radius [nm]	8.72
Indent surface	(001), (111)
Pushing speed [m/s]	1.0
Maximum depth [nm]	5.0

Extended CNA analysis



DXA analysis[3]



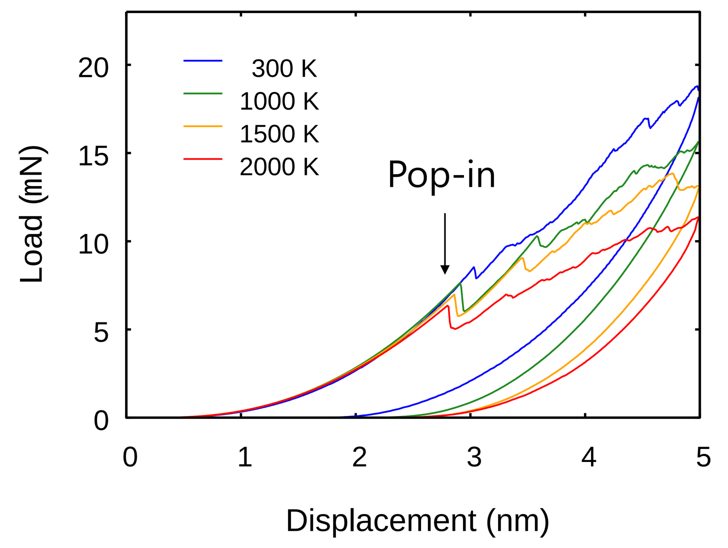
SiC crystal structure is composed of the superposition of Si and C sublattice. After removing C atoms, CNA (Common Neighbor Analysis) is applied to Si sublattice. DXA (Dislocation Extraction Algorithm) identify all dislocations in crystal, determine their Burgers vectors, and output dislocation lines.

[3]A. Stukowski *et al.*, Modelling Simul. Mater. Sci. Eng. **20**, 085007 (2012).

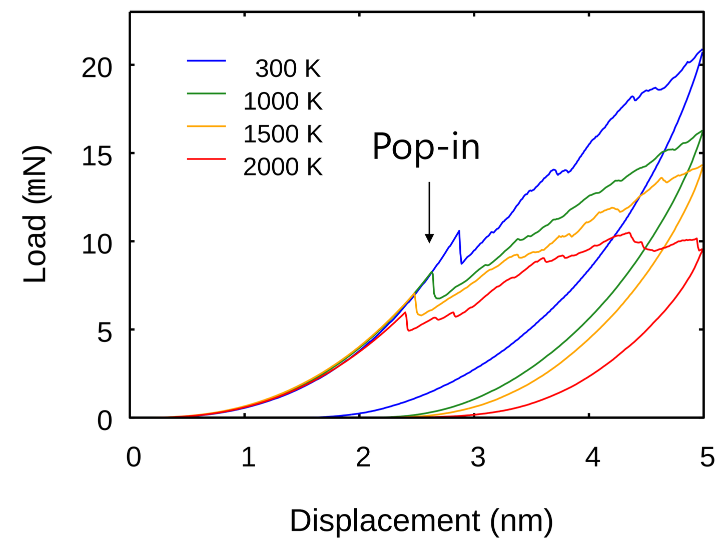
Results and discussion

Load – displacement curves

(001) indent



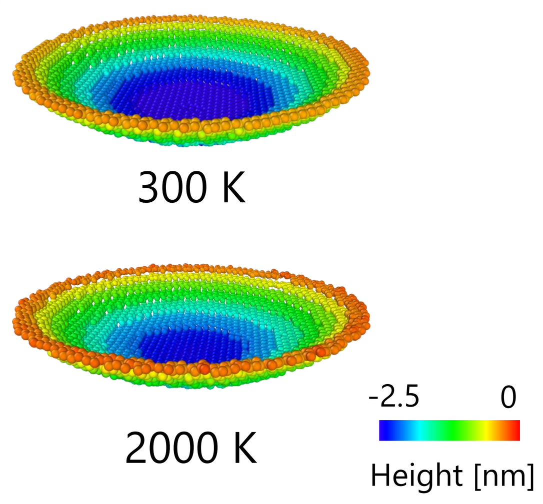
(111) indent



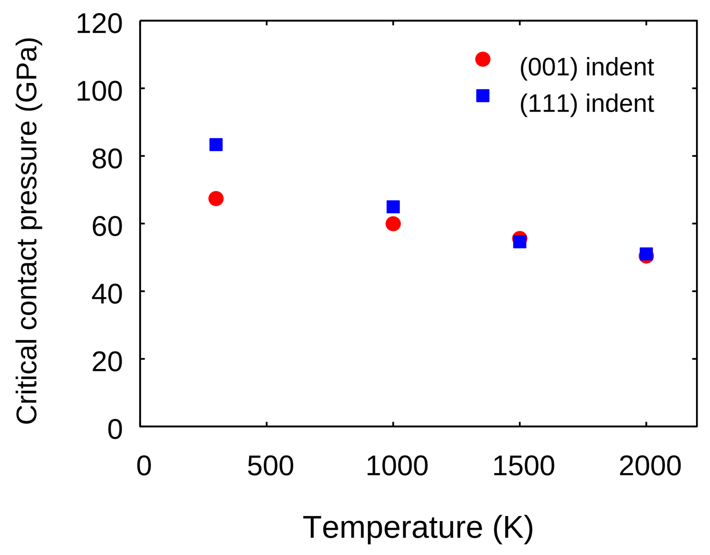
Transition from pure elastic to elastic-plastic deformation, known as pop-in event, is observed. Elastic response does not depend on temperature. In contrast, elastic-plastic curves shift downward with increasing temperature.

Pop-in contact atoms

(111)



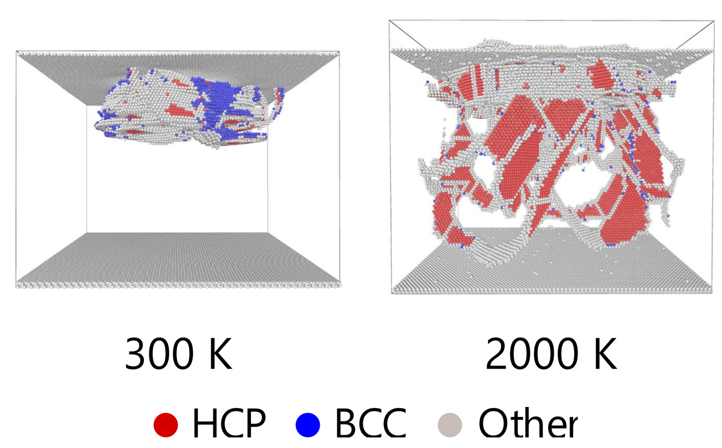
Pop-in criteria



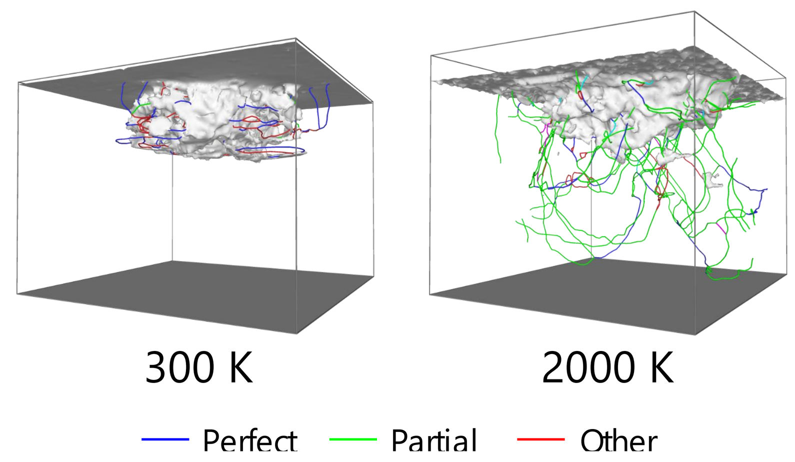
Projected contact surface is circle even at high temperature. (111) plane has higher resistance against plastic deformation than (001) at lower temperature.

Characteristics of lattice defects, (111)

Extended CNA



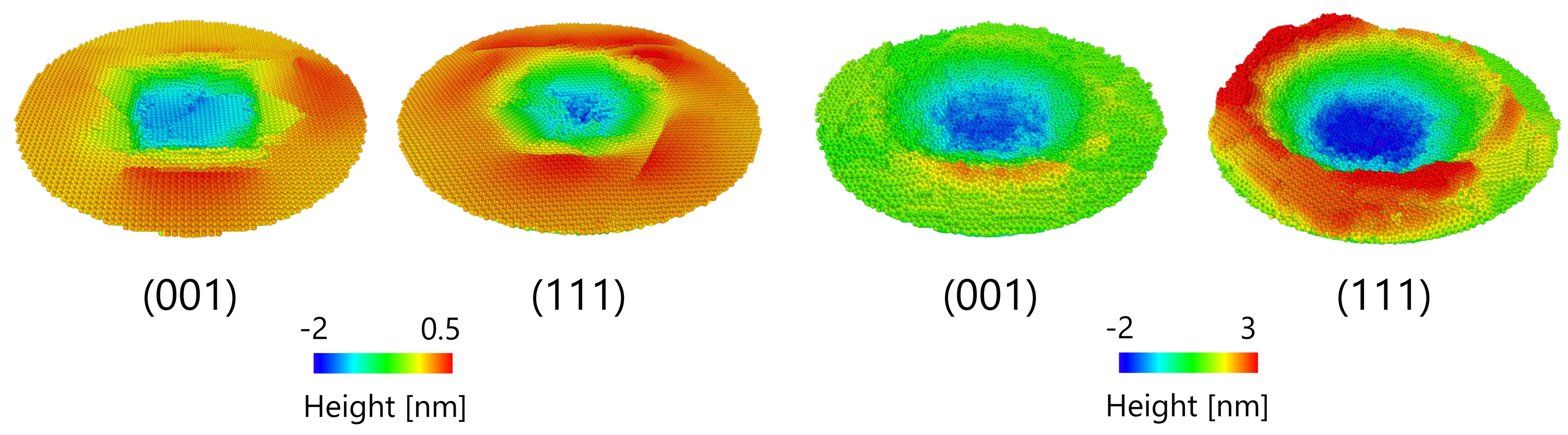
DXA



Perfect dislocations are dominant at low temperature, whereas partial dislocations with stacking faults dramatically increase at high temperature.

Impressions after nanoindentation

300 K   2000 K



Pileup pattern for (001) and (111) indent have four and six-fold symmetry, respectively, at low temperature. On the other hand, at high temperature such symmetry disappear and larger pileups are formed.