Indentation of Silicon: Phase Transition?


Cut away of crystalline Si indented with a tetrahedral indenter.

**FOCUS:** MD simulations to elucidate 2 phase transitions of Si; diamond $\rightarrow$ β-Sn (exp), diamond $\rightarrow$ thermodynamically unfavorable amorphous phase. Many-body Si potential used, was developed by Stillinger and Weber (*Phys. Rev. B* 31, 5262-5271 (1985)).

**CONCL:** Although amorphous Si did not undergo phase transition to solid, crystalline Si $\rightarrow$ amorphous phase near the indenter, No transition to β-Sn. Lower yield strengths near melting temp and slow indentation speeds.


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Indentation of Silicon: Phase Transition?


**MD: NVT 350,000 atoms**

**CONCL:** Tip-Substrate: Morse potential

$v=40$ m/s


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Indentation of Silicon: Phase Transition?

Blue = cubic Si (4 neighbors)
Red = β-Si (6 neighbors)


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Indentation of Silicon: Phase Transition?

Flattening of Tetrahedron upon indentation

- withdrawal of tip leads to amorphous phase
- repeated indentation leads to a mixture of the β (distorted) and amorphous phases

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Multiscale Simulations of Si Indentation

2D: Infinite cylinder
3D: Spherical Indenter

Local quasicontinuum method (Tadmor, Ortiz, Phillips) using Stillinger Weber potentials and non-orthogonal tight-binding Hamiltonian (Bernstein & Kaxiras)


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Both SW & TB differ from DFT curves!

In 3D, see bct5, β-Sn, sc & bcc under the indenter.
Multiscale Simulations of Si Indentation

In 3D, see bct5, β-Sn, sc & bcc under the indenter.

Force curves compare well with experiment but not phase transition behavior!

Some other Si work:

Indentation of Diamond using a sharp tip

REBO potential used for MD simulations of indentation and pull-back of sp³-hybridized carbon tip and hydrogen terminated diamond substrate

Figs show initial indentation, maximum compression, pull-back and transfer of material, to final zero-load with material transfer
- Tip twisted during indentation, to minimize repulsions.
- Twisting caused bonding between tip and diamond substrate.
- Retracted tip subsequently deformed, due to twisting
- Material transfer between tip and film
Indentation using Sharp Tips

Indent [111]

**SWNT**: Rigid or Flexible (10,10)

**DWNT**: Flexible

Diamond Counterface

C_{13} (2x2)

X (perpendicular to chain tilt)

Y (parallel to chain tilt)

Sliding speed = 100 m/s
Slide duration = 40 ps
time step = 0.25 fs
Temp = 300 K
AIREBO Potential

C_8, C_{13}, C_{22}

Flexible versus Rigid nanotube tips

Force curves using different tips


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Structure factor equations

Carbon atoms of C$_8$ chains closest to nanotube

Before Indentation: Separation 2.0 Å
After Some Indentation: Separation ~5.5 Å

a and b are unit cell vectors
Distinct domains form as a result of the indentation.

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Elastic constants for Alkane Monolayers


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Compression of Alkylsilane Monolayers


Courtesy of: M. Chandross, E.B. Webb III, M.J. Stevens, G.S. Grest
Sandia National Laboratories, Albuquerque, NM
Compression of Alkylsilane Monolayers


- Alkylsilane monolayers bonded to substrate
- Crystalline substrate
- Chains with n= 6, 8, 12, 18 carbons in backbone
- All-atom molecular dynamics simulation
- LAMMPS MD code

Courtesy of: M. Chandross, E.B. Webb III, M.J. Stevens, G.S. Grest
Sandia National Laboratories, Albuquerque, NM

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Compression of Alkylsilane Monolayers


- Shorter chains stiffer than longer (agrees with hydrocarbon chains)
- Strength of attractive minimum ~ 140MPa in agreement with experiment

Courtesy of: M. Chandross, E.B. Webb III, M.J. Stevens, G.S. Grest
Sandia National Laboratories, Albuquerque, NM
Salmeron Tribol. Lett. 10 (2001) 69
Indentation of amorphous carbon films
*varying hydrogen content*

Gao, et. al., in preparation

Compression of alkyne SAMs with an amorphous carbon tip

Perpendicular-chain system
(56 chains at 300 K)

-\text{C}_8\text{H}_{16} - \text{C} \equiv \text{C} \equiv \text{C} - \text{C}_8\text{H}_{17}

End-chain system
(56 chains at 300 K)

-\text{C}_{14}\text{H}_{28} - \text{C} \equiv \text{C} \equiv \text{C} - \text{C}_2\text{H}_5

Polmerization occurs in all systems

End-chain monolayer

-\text{C}_{14}\text{H}_{28} - \text{C} \equiv \text{C} \equiv \text{C} - \text{C}_2\text{H}_5

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