Size Effects in Nanoscale Wear of Silicon Carbide and Silicon

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Why study tribology (friction, adhesion and wear)?

Frequently occurs in daily life in the form of energy consumption, machine wear, cutting, …

K. Holmberg et al, Tribology International 47, 221–234,(2012)
Why study with AFM

Atomic force microscopy (AFM) makes it possible to probe properties at nanoscale with more precise control parameters such as load, displacement.

Engineering rough surface at different scale

Suppress fracture\(^1\) and Improve machinability\(^2,3\):
- Reduction of deformation zone to nanoscale regime suppresses fracture

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Study of nanoscale wear of SiC

Q1: What is the nanoscale wear behavior in the plastic deformation regime of SiC?

Q2: Do the wear mechanisms of SiC differ between the micro- and nanoscales?

Wear resistance of materials

Archard’s equation\(^1\)

\[
\text{Wear volume} = \frac{k \times \text{Load} \times \text{sliding distance}}{\text{Hardness}}
\]

\[
k = 10^{-2} - 10^{-8}
\]

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Hardness of materials

<table>
<thead>
<tr>
<th>Sample</th>
<th>Hardness (GPa)</th>
<th>Elastic modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>sc-SiC (4H-SiC with an orientation of (0001) ± 0.5°)</td>
<td>37±1</td>
<td>397 ± 8.5</td>
</tr>
<tr>
<td>nc-SiC nanocrystalline 3C-SiC, (111) orientation</td>
<td>26±2</td>
<td>292 ± 36</td>
</tr>
<tr>
<td>Si (p-type, (100))</td>
<td>12.6±0.2</td>
<td>160 ± 5</td>
</tr>
<tr>
<td>SiOₓ (Native oxide)</td>
<td>8(1)</td>
<td>73(1)</td>
</tr>
</tbody>
</table>

- Hardness of nc-SiC is lower than of sc-SiC.
- Hardness of SiC is 3 times as large as of Si.

According to Archard’s equation, SiC is expected to have less wear than Si.

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Scratching with nanoindentation

Experimental parameters:
Berkovich diamond tip with a radius of 370 nm at humidity ~ 3%, 500 cycles

As expected, harder material has less wear.
Scratching with AFM

- **e** sc-SiC at 600 nm
- **f** nc-SiC at 600 nm
- **g** Si at 120 nm
- **h** SiO\textsubscript{x} at 400 nm

Graphs showing height and max scratch depth vs. applied load for sc-SiC, nc-SiC, Si, SiO\textsubscript{x}.
Wear resistance is no longer simply correlated with hardness in nanoscale contacts.

Qualitative contribution to friction and wear

Nanoindentation (R ~ 370 nm)

AFM (R ~ 20 nm)

Tip

Sample

Plastic zone

Transition due to the plastic zone size

Hardness

Adhesion/Interfacial shear strength

Wear volume (V) = f (H)

V = f (H, surface chemistry)

Need models to describe this relation
SiC may or may not outperform Si, but it depends on the contact size and load regime.

We found a switching of the relative wear resistance for SiC and Si as the nanoscale contact size is reduced even when plastic zone is well developed.

At the nanoscale, material hardness is not the only factor that governs wear resistance. Surface chemistry effects on plastic deformation need to be taken into account in order to predict wear behavior.
Thank you!

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Atomic force microscopy (AFM) makes it possible to probe properties at nanoscale with more precise control parameters such as load, displacement.

**Engineering rough surface at different scale**

Manufacturing in nanoscale contacts

: Formation of ductile chips with lower cutting forces in SiC

Nanoscale wear of silicon carbide

Properties of SiC

- High temperature stability
- Good corrosive resistance
- High hardness and elastic modulus
- Thin coating capability

1. Silicon Carbide Ceramics Abrasion Protection and High Temperature Resistance Linings from Kalenborn company
2. SiC coating components from Entegris company
3. Polycrystalline SiC MEMS (UC Berkeley)

Scratching with nanoindentation

Relative wear resistance = \frac{\text{Load} \times \text{Sliding distance}}{\text{Wear volume}}

As expected from Archard’s equation, harder material has more wear resistant.
Scratching with AFM

Experimental parameters:

Humidity <3%
2400 cycles
Nanocrystalline diamond tip with a radius of:
$R_{\text{SiC}} = 22\pm7 \text{ nm}$,
$R_{\text{Si}} = 13\pm4 \text{ nm}$,
$R_{\text{SiO}_x} = 17\pm3 \text{ nm}$

Harder material does not necessary has less wear.
Transition of wear regime

Nanoindentation (R ~ 370 nm)

Wear resistance of SiC is better than Si.

AFM (R ~ 20 nm)

Wear resistance of Si is better than SiC.

Q: Why relative wear resistance ability is switched?
Qualitative contribution to friction and wear

Nanoindentation (R ~ 370 nm)

AFM (R ~ 20 nm)

Transition due to the plastic zone size

Friction

\[ F_f = F_{\text{plowing}} + F_{\text{shear}} \]

Plastic deformation
Interfacial chemistry

Contact size

Interfacial chemistry
Plowing


We have to demonstrate that

- In nanoindentation, plastic zone size is more developed and therefore, more plowing contribution (hardness) in this case.

- In AFM, when shear contribution is dominated, interfacial shear strength (Larger resistance to sliding) of sc-SiC and nc-SiC should be higher than Si and SiO\textsubscript{x} in order to both SiCs to have higher wear in this regime.
Testing hypothesis

Size of the plastic zone

Interfacial shear strength

Plastic zone size is more developed under nanoindent tip.

Interfacial shear strength of sc-SiC and nc-SiC are indeed higher than of Si and SiO$_x$. 

Nanoin indentation

Interfacial shear strength (MPa)

Material

sc-SiC  nc-SiC  Si  SiO$_x$
New phenomena at nanoscale regime

Wear via atom-by-atom removal\(^1\) (atomic attrition)

Wearless phenomena - negative friction coefficient\(^2\)

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Plays a role

Friction and wear is a complicated process.

- Environment
  - Atmosphere
  - Humidity
  - Temperature

- Process parameters
  - Load
  - Velocity
  - Tip geometry

- Material property
  - Hardness
  - Toughness
  - Strength

- Interface property
  - Roughness
  - Surface chemistry
  - Lubrication

Many tribological problems are still best approached through empirical investigations.
Size of the plastic zone

Nanoindent tip
50 - 2000 µN
R ~ 370 nm

AFM tip
120 – 3500 nN.
R ~ 17-22 nm

\[
\frac{E}{\sigma_y} \tan \beta = 6(1 - \nu) \left(\frac{c}{a}\right)^3 - 4(1 - 2\nu)
\]

Plastic zone size is more developed under nanoindent tip.

Wearless: interfacial shear strength

Before

After

Friction

Shear strength (τ)

Load

Friction (nN)

Applied load (nN)

Negative regime

Positive regime

sc-SiC

nc-SiC

Si

SiO₂

26
Interfacial shear strength of sc-SiC and nc-SiC are indeed higher than of Si and SiO$_x$. 
Effect of roughness on shear strength

Effect of roughness on interfacial shear strength in this scale is insignificant

<table>
<thead>
<tr>
<th>Sample</th>
<th>Roughness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>sc-SiC</td>
<td>0.19±0.08</td>
</tr>
<tr>
<td>nc-SiC</td>
<td>0.58±0.26</td>
</tr>
<tr>
<td>Si</td>
<td>0.070±0.002</td>
</tr>
<tr>
<td>SiO_x</td>
<td>0.16±0.01</td>
</tr>
</tbody>
</table>

Higher roughness → Less contact area → Less friction

Effect of surface chemistry on shear strength

Surface chemistry is responsible for the different in interfacial shear strength

<table>
<thead>
<tr>
<th>Sample</th>
<th>Oxide thickness (nm)</th>
<th>Type of oxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>sc-SiC</td>
<td>3.16</td>
<td>SiO$_2$, Si$<em>4$C$</em>{4-x}$O$_2$</td>
</tr>
<tr>
<td>nc-SiC</td>
<td>1.81</td>
<td>SiO$_2$, Si$<em>4$C$</em>{4-x}$O$_2$</td>
</tr>
<tr>
<td>Si</td>
<td>3.62</td>
<td>Si, SiO$_2$</td>
</tr>
<tr>
<td>SiO$_x$</td>
<td>16.20</td>
<td>SiO$_2$</td>
</tr>
</tbody>
</table>
1. Background: Tribology

2. Research projects:
   I. Nanoscale wear of silicon carbide. (Published)
   II. Mechanical properties and creep behavior of ultra-stable organic glasses. (Manuscript in preparation)
   III. Deformation of vapor-deposited and melt-quenched metallic glass (Propose)

3. Summary
Mechanical properties and structure

TPD : N,N’- Bis(3-methylphenyl)-N,N’ diphenylbenzidine

Pixel array fabricated on flexible PEN plastic substrate.\(^1\)

Roll-to-roll deposition of organic films on foil.\(^1\)

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Key points

- The values were averaged between 20-45 nm of contact depth.
- For reduced elastic modulus, there is a maximum trend around 310 K.
- For hardness, there is a maximum trend around 280 K.

Hypothesis

- Correlation between elastic modulus and orientation of TPD glasses.
- Correlation between hardness and density of TPD glasses.
Elastic modulus on orientation of molecule

Key point
- Elastic modulus depends on the orientation of molecule. (Max increase ~29%)
- Hardness depends on the density. (Max increase ~ 47%)
Creep analysis

Key point

- Creep ratio of vapor-deposited glass depends on deposition temperature.
- Hardness and creep ratio are inversely correlated. That means creep plays an important role in determining mechanical properties of vapor-deposited TPD glass.

PVD can control structure of thin film and manipulate mechanical properties and creep behavior.
1. Background: Tribology

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3. Summary
What is metallic glass?

A metallic material which has a disordered atomic-scale structure (also called amorphous metal)

The advantages of metallic glass

1. High specific strength
2. High hardness
3. High elasticity
4. Forming ability
5. Near net shape
6. Corrosion resistance
7. Wear resistance

Advantage of PVD method

Improvement of stability and physical properties

• Low enthalpy
• Higher density

Improvement of mechanical properties

• Higher hardness
• Higher elastic modulus

Metallic glass as coating material

Archard’s equation

\[
\text{Wear volume} = \frac{k \times L \times S}{\text{Hardness}}
\]


Yugeswaran, S. et al. Vacuum, 2014 (110), 177-182
Wear resistance of metallic glass

Wear correlate with hardness.

Load (µN)

Average depth (nm)

Critical range

Highest hardness

Hardness (HV)

Volume Loss (mm³)

Crystallized Volume Fraction (%)

Volume Loss (20N)

Hardness

CZT

CZTA

CZTB


Wear does not correlate with hardness. It is thought to be related to the wear mechanism.

Louzguine-Luzgin, D. et al. Materials Letters, 2016 (185), 54-58,
Fracture toughness on wear of metallic glass

Hardness (H), Yield strength (σ_y), Elastic modulus (E), Glass transition temperature (T_g), the notch toughness (K_Q) and the Poisson's ratio (ν) of BMGs do not independently exhibit a direct correlation to the specific wear rate.

The wear resistance is dominated by synergistic effects of strength factors and toughness factors.
Q1: What are the differences between the relative wear resistance properties of vaper-deposited metallic glass and melt-quenched metallic glass?

Q2: What are the mechanisms that control friction and wear between these two metallic glasses with different tip sizes?
Wear test will be done by AFM and Nanoindentation. Scratch or indents morphology will be done by AFM and SEM. Fracture toughness will be done by Nanoindentation. Strength will be done by simulation of tensile test by LAMMPS. Surface chemistry will be done by XSP.
Q3: What level of heterogeneity controls mechanical and wear resistance properties in vapor-deposited glass?

Icosahedral (ICO) order in CuZrAl corresponds to higher local stiffness and yield resistance (stability), while shear transformation preferentially nucleates from more disordered regions.

Heterogeneity in a metallic glass

Amplitude-modulation atomic force microscopy (AM-AFM)

Hyperquenched metallic glass
Relaxed at 553 K for 5 min
Relaxed at 553 K for 720 min

Nanoindentation modulus map

Proposed questions to be addressed.

Q1: What are the differences between the relative wear resistance properties of vaper-deposited metallic glass and melt-quenched metallic glass?
   - Wear test by Nanoindentation and AFM.
   - Wear debris observation by AFM and SEM.

Q2: What are the mechanisms that control friction and wear between these two metallic glasses with different tip sizes?
   - Fracture toughness by Nanoindentation.
   - Strength by Molecular dynamics simulation of tensile deformation.
   - Crack morphology by AFM and SEM.

Q3: What level of heterogeneity controls mechanical and wear resistance properties in vapor-deposited glass?
   - Molecular dynamics simulation using LAMMPS for tensile test.
   - AM-AFM mapping or modulus mapping by AFM.
   - Modulus mapping by Nanoindentation.
Conclusion

Research projects:

1) Nanoscale wear of silicon carbide.
   • Tool size does indeed affect the wear resistance properties
     and it can change the domination mechanism.

2) Mechanical properties and creep behavior of ultra-stable organic
   glasses.
   • We can tune structure in a way that can control
     mechanical properties by PVD techniques.

3) Deformation of vapor-deposited and melt-quenched metallic
   glass.
   • We will investigate the relationship among wear
     resistance properties, microstructure, and tip size.