Hydrogen/Argon Plasma-Amorphous Carbon Near-Surface Interactions

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Overview

- Monitoring H\(_2\) and Ar plasma erosion of a-C:H films using both molecular dynamics (MD) simulation and in-situ ellipsometry

- Study the role of plasma parameters such as a) ion energies, b) ion/neutral flux ratio, c) ion flux composition and d) electron and UV fluxes/energies, on influencing the near-surface region chemistry and etching mechanisms.

- Study the reaction mechanisms which dominant the etching process

- This work is in collaboration with the experimental group at the University of Maryland, who is working on real-time ellipsometric measurements
**Initial Conditions**

- **α-C:H film:**
  - Dimension: 2.8x2.8x7.5 nm
  - H content: 27%
  - Sp3 bonding: 25.4%
  - Density: 2.4 g/cm³
  - Bottom 2 layers fixed
  - Surface temperature: 300K

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Top view

Side view
Parameters to study

- Plasma parameter & H concentration in the initial film:
  - Case I: Ar$^+$ interaction with a-C:H film with 50-200eV impact energy
  - Case II: H$_2^+$ interaction with a-C:H film with 50 eV impact energy
  - Case III: H$_2^+$ interaction with pure a-C film with 50 eV impact energy
Case I: Ar⁺ interaction with α-C: H film
With increased ion energy, the modified layer thickness is larger.

- The hydrogen concentration (%) of the modified layer decreases as the ion energy increases - Higher energy ions deplete H in the surface region more effectively during steady state
- Our MD simulations results are in good agreement with experimental results describing Ar+ erosion of a-C:H for -50V, -100V and -200V bias cases
Case II: $\text{H}_2^+$ interaction with $\text{a-C:H}$ film
The near-surface film structure and composition under steady state conditions is the result of a competition between erosion and insertion processes.
Impact energy: 50 eV
8000 impacts in total (equivalent to fluence of $9.9 \times 10^{16} \text{cm}^{-2}$)
a-C:H Film composition after H$_2^+$ impacts

Impact energy: 50 eV
8000 impacts in total (equivalent to fluence of 9.9x$10^{16}$cm$^{-2}$)

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<th>C composition</th>
<th>H composition</th>
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```

Original film
The affected surface initially expands due to the chemical modification.
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2.5 nm modified layer was formed after 8000 impacts (fluence~$10^{17}$ cm$^{-2}$), with C:H ratio close to 1.

Around 1.5 nm thick film was etched away.
Case III: H$_2^+$ interaction with a-C film
Impact energy: 50eV
Film dimension: 2.8x2.8x4.7nm
5000 impacts (equivalent to fluence of $6.2 \times 10^{16}$ cm$^{-2}$)
a-C Film composition after H$_2^+$ impacts

Impact energy: 50eV
Film dimension: 2.8x2.8x4.7nm
5000 impacts (equivalent to fluence of 6.2x10$^{16}$cm$^{-2}$)

Original film surface
The affected surface initially expands due to the changing chemistry.
The affected surface initially expands due to the changing chemistry. A 2.5 nm thick modified layer with C:H ratio close to 1 was formed after 5000 impacts. This modified layer thickness and composition does not depend on the initial H concentration of the material.
The plasma modifies the film by depleting or saturating the surface of hydrogen.

Modified layer thickness and composition does not depend on the H concentration in the initial material. It is dependant on ion energy and composition:

• With Ar\(^+\) impacts, the modified layer thickness increases with increasing impact energy. The H concentration of modified layer decreases with increasing impact energy. The modified layer is carbon rich film due to the depletion of the H during the ion impact.

• With H\(_2\)^+ impacts, the film expands initially due to the polymerization of the near-surface region. The modified layer with C:H ratio of 1, is around 2.5 nm.