Erosion Mechanism of Amorphous Hydrocarbon Film by H\textsubscript{2} Plasma: A Molecular Dynamics Simulations Study

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ABSTRACT

The goal of this study is to mimic etching process in order to better understand plasma-surface interactions. The erosion mechanisms of H\textsubscript{2} plasmas interacting with a-C:H surfaces was studied using molecular dynamics simulations based on reactive empirical bond order (REBO) potential. The preliminary study has indicated the influence of plasma parameters (energies, ion/neutral flux ratio, and ion flux composition) on reaction mechanism. The chemical reactions of H\textsubscript{2} with a-C:H surfaces were identified by analyzing trajectories obtained from molecular dynamics calculations. The relation between film composition, sputtered products, erosion rate and plasma parameters will also be discussed.

COMPUTATIONAL METHODOLOGY

A reactive empirical bond order potential [1-3] was employed to simulate the plasma-surface interaction for our study. The details of the simulation methods is described in Ref [4].

● Configuration of a-C:H film:
  - Dimension: 2.8x2.8x4.5 nm
  - Surface temperature: 300K
  - H content: 26%
  - sp3 bonding: 21.4%
  - Bottom two layers fixed

● a-C:H film structural properties:
  - Radial distribution function
  - Composition depth profile
    - Carbon-rich film with the constant hydrogen concentration through the layers.
  - Initial impact conditions:
    - Ar impacts:
      - Impact energy: 50-300 eV
      - a-C:H surface dimension: 1.4 x 1.4 x 3.9 nm
      - 3000 impacts – 1.5e+17 cm\textsuperscript{-2} Ar fluence
    - H\textsuperscript{+} impacts:
      - Impact energy of H\textsuperscript{+}: 50, 100 eV
      - Internal temperature of H\textsuperscript{+}: 0 K
      - Impact energy of H: 0.1 eV
      - Ratio of H/H\textsuperscript{+} ranges from 0 to 100
      - 5000 impacts – 6.2e+16 cm\textsuperscript{-2} H\textsuperscript{+} fluence
      - Surface cools back to 300 K by the end of each impact

References

RESULT AND DISCUSSION

● Effects of Ion Energy:
  - Collision tree of Ar interactions with a-C:H film
  - Ion/neutral flux ratio VS treated a-C:H film composition
  - Composition depth profile
    - RHEED: Range = 10
      - H\textsuperscript{+} impact energy: 50 eV
      - The affected surface expands initially due to the changing chemistry.
      - The film composition remains a steady state.
      - Top of the film is hydrogen rich.
      - H\textsuperscript{+} and C concentration become equal at around 10 Å from the surface.
      - H\textsuperscript{+} impact energy: 50 eV
    - The affected surface expands initially due to the changing chemistry.
  - Ion energy VS sputter yield

CONCLUSION

The influence of ion energy and ion/neutral flux ratio on interaction of light species with a-C:H film was studied:
I. Higher ion energy causes higher etching rate.
II. In the case of H\textsuperscript{+} flux, higher neutral ratio leads to less important etching rate, which is due to the important role of H\textsuperscript{2}+ in the etching process. H\textsuperscript{2}+ not only breaks C-C or C-H bond in the film (on the surface and in depth), but also increases hydrogen content in the film, which leads to the polymerization of the amorphous film, and depletion of those polymer chains.
The dominant sputtered species (CH\textsubscript{3}, CH\textsubscript{2}, C\textsubscript{2}H\textsubscript{4}, C\textsubscript{2}H\textsubscript{2}, CH) are not dependent on ion/neutral flux ratio, nor on impact energy, and they are very reactive species. The average temperature of the sputtered species is above room temperature.