MD simulation study on CN passivation film formation on organic polymer surface

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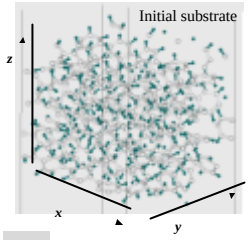
Background of the study

- **Need of low-k materials as insulator in microfabrication of semiconductors**
  - organic polymers are candidates for such insulating materials
- **Development of inter-atomic potential functions**
  - the functions used for MD simulations of (H,C,N) system proposed by Yamada and Hamaguchi
    (Yamada and Hamaguchi; JSAP spring meeting 2004; preprint)
- **Prior MD simulations of (H,C) system**
  - H atoms injected break chemical bonds of organic polymer substrates and C atoms are deposited on the substrate surface forming amorphous carbon layers
  - speculation ; N atoms also form rigid masks on the substrate surface of organic polymer, i.e., CN mixing layers

Preparation for MD simulations

- **Poly(1,4-phenylene) (PPP) is chosen as a simple model of organic polymer**
  - destruction of benzene rings may be essential for etching process of organic polymer substrate
- **Modification of some parameters of inter-atomic potential functions**
  - some parameters associated with N atoms of Yamada 's potential functions are modified so as to represent more realistic chemical bonds including N atoms

PPP substrate



— **Poly(1,4-phenylene) as a model substrate reproducing the mass density* 1.33 g/cm^{-3}**

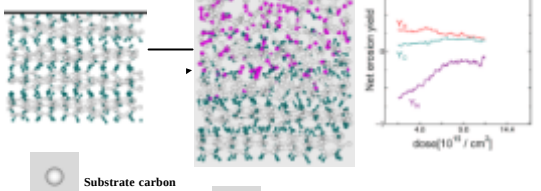
— **Cross sectional area of the simulation box is about 4 nm^2.**

— **Periodic boundary conditions are imposed to the horizontal (*x* and *y*) directions.**

— **Incident molecules,**
C, N, N_2, N_2H,
are *vertically* injected.

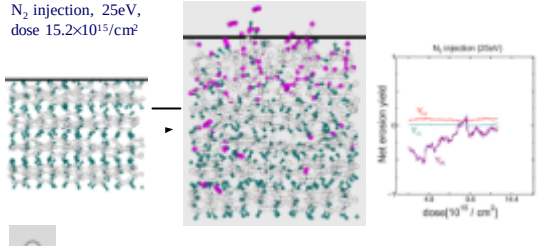
Particle injection 1

N injection, 25eV,
dose 14.4×10^{15}/cm^2



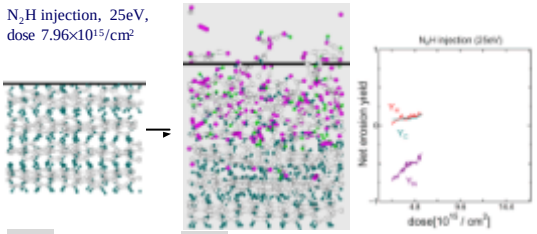
Particle injection 2

N_2 injection, 25eV,
dose 15.2×10^{15}/cm^2



Particle injection 3

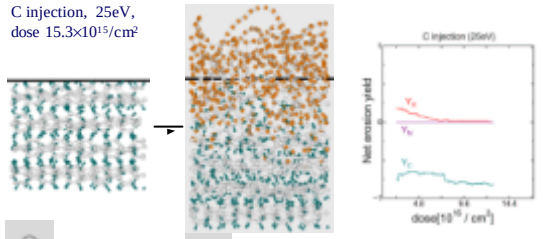
N_2H injection, 25eV,
dose $7.96\times10^{15}/cm^2$



Substrate carbon
Substrate hydrogen
Injected nitrogen
Injected hydrogen

Particle injection 4

C injection, 25eV,
dose $15.3\times10^{15}/cm^2$



Substrate carbon
Substrate hydrogen
Injected nitrogen
Injected hydrogen
Injected carbon

Findings

- **With N atom injections, a CN mixing layer is observed to be formed.**
- **For N_2 and N_2H injections, CN mixing occurs although formed films are somewhat weaker than those in N injections case**
- **Injected C atoms are observed to form amorphous carbon layers on the substrate with the new inter-atomic potential functions as in the case of Brenner's functions.**
  (H. Yamada and S. Hamaguchi, J. Appl. Phys. 96 (2004) 6147)