Simulation of Plasma Processing with FPS3D

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Simulation of plasma processing via a Monte Carlo feature-scale simulator FPS3D is demonstrated by two very different examples: simulation of etching and implantation for the case of Ar/Cl_2 plasma, and simulation of atomic layer deposition with a cyclic process of dichlorosilane gas followed by the ammonia plasma. Comparison with experiments is provided.

1. Introduction - FPS3D.

Feature-scale simulations allow reasonably fast simulation of etching or deposition profiles. These simulations are many orders of magnitude faster that the higher accuracy MD methods. There have been many types of feature-scale simulators developed since the 1970s, and their capabilities differ significantly from each other.

FPS3D is a general software package designed to be applicable to any situation met by the semiconductor industry, be that etching, deposition, implantation, atomic layer processing, etc., or any combination of these. FPS3D uses a cellular model for representing solid materials, but that model goes well beyond the traditional approach. In FPS3D, each cell can contain different molecules and the number of molecules per cell is not fixed but rather is determined by the volume of the cell and by the size of molecules it contains. Also, FPS3D uses Monte Carlo pseudo-particles for representing all incoming fluxes. These particles are launched such that statistically they represent given angle-energy distributions of all relevant fluxes of species coming to the surface. Each particle typically contains many molecules, but preferably significantly fewer than the number of molecules in a full cell. Upon collision of such a particle with a solid material, the code determines a set of involved cells where interactions occur and computes the output on the basis of user-specified reactions.

FPS3D is free from many limiting assumptions of most other feature-scale simulators. For etching it allows simultaneously calculation or implantation, and for deposition, it allows materials to grow in accordance with their density, and in accordance with the actual sizes of participating molecules.

2. Two Examples of FPS3D Simulations

FPS3D can be applied to features of different scales ranging from nanometers[3] to microns[2]. By selecting proper sizes of material cells and incoming particles, the code obtains reasonable accuracy within reasonable calculation time.

2.1. Etching/Implantation with Ar/Cl_2 plasma

To setup surface reactions for the case of Ar/Cl_2 plasma etching of Si, FPS3D was run with the low ion energies of 35, 55 and 75 eV. Results of simulations were able to reproduce the experimental data[4]. High-aspect ratio etching often requires high-energy ions. We have used the same chemistry for the case with high energy Ar+ ions of 1.5 keV. Energetic ions penetrate deep into material, and sometimes could lead to plasma-induced damage. We simulated this process both in 2D and 3D.

2.2. SiN Atomic Layer Deposition with Cycles of Dichlorosilane and Ammonia Plasma

We considered a case of SiN ALD that uses cycles of dichlorosilane gas deposition followed by the nitration by ammonia plasma. This case is interesting because it results in the deposition of 1 ML only after two cycles. We believe that one of the main reasons for this is steric hindrance by SiH_2Cl_2 molecules. FPS3D is designed to take steric hindrance into account. This large molecule could cover two interaction sites on the surface, preventing those sites from interacting with other molecules until the large molecule reacts and reaction sites become accessible again. Results of simulations are compared with experiments[5].

References

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