【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Interdisciplinary Science and Engineering)

Title of Project : Quantum Theoretical Analyses of Plasma Processing for Novel and Diverse Materials Using Multi-Scale Numerical Simulations

Satoshi Hamaguchi
(Osaka University, Graduate School of Engineering, Professor)

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Research Area : Plasma Electronics
Keyword : Numerical Simulation, Plasma Surface Interaction, Plasma Process

【Purpose and Background of the Research】

Material surface modification by plasma has been widely used for various applications such as semiconductor device manufacturing and biomaterial surface conditioning. Recently non-thermal equilibrium chemical reactions under low-energy ion impact are typically used for such processes as they typically require low damage processing. However, some of such surface reactions are not well understood in the traditional framework of plasma processing, where energetic ion incidence plays a major role. The goal of this study is, therefore, to clarify low-incident-energy non-thermal equilibrium surface chemical reactions during low-damage plasma processing, using quantum mechanical analyses of interactions between incident species and the surface materials. Even under the conditions of low-energy ion incidence, dynamics of incident species interacting with a large number of surface atoms need to be simultaneously analyzed. Therefore multi-scale analyses that connect atomic-scale dynamics to macroscopic dynamics are needed for a better understanding of the surface phenomena.

【Research Methods】

The multi-scale numerical simulation that this study aims to achieve includes quantum-mechanical (QM) simulation, classical molecular dynamics (MD) simulation, particle-in-cell (PIC)/Monte-Carlo (MC) plasma simulation, and fluid-model plasma simulations, as illustrated in Fig. 1. Simulation results will be compared with plasma and beam experiments that will be also performed in this study.

【Expected Research Achievements and Scientific Significance】

With the multi-scale simulation system, we plan to clarify surface chemical reaction mechanisms during processing of metal oxides and other new materials used in the latest microelectronics devices as well as biomaterials that have been widely used in regenerative medicine recently.

Figure 1 Outline of Multi-Scale Simulation System that we plan to construct in this research project.

【Publications Relevant to the Project】

・K. Mizotani, *et al.,* "Molecular dynamics simulation of silicon oxidation enhanced by energetic hydrogen ion irradiation," J. Phys. D: Appl. Phys. **48**(15) (2015) 152002 (5pp)
・H. Li, *et al.* "Suboxide/subnitride formation on Ta masks during magnetic material etching by reactive plasmas," J. Vac. Sci. Tech. A **33**(04) (2015) 040602 (5pp) ..
・K. Karahashi and S. Hamaguchi, "Ion beam experiments for the study on plasma-surface interactions," J. Phys. D: Appl. Phys. **47**(22) (2014) 224008-1~224008-15.

【Term of Project】 FY2015-2019

【Budget Allocation】 116,900 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.camt.eng.osaka-u.ac.jp/hamaguchi/
hamaguch@ppl.eng.osaka-u.ac.jp