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Semiconductor Process Simulation Studies by ReaxFF Molecular Dynamics Methods: Applications for Chemical Vapor Deposition and Atomic Layer Deposition Processes

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ABSTRACT

Semiconductor devices support state-of-the-art technologies such as automated driving, the Internet of Things (IoT), and big data. Chemical vapor deposition (CVD) and atomic layer deposition (ALD) are common and powerful technologies for growing a high-quality thin film for advanced semiconductor devices. The film properties strongly depend on the process parameters such as substrate temperature, gas composition, pressure, exposure time, etc. Therefore, understanding these relationships is essential to obtain the desired properties. Many experimental trials and errors have been reported; however, multiple process parameters are tough to optimize and elucidate the atomic scale mechanisms. Numerical simulations are reasonable solutions by constructing models that can appropriately reproduce natural phenomena on that time-spatial scale. I aim to elucidate the fundamental mechanisms on the surface in atomic scale in the semiconductor processes, using reactive force-field molecular dynamics (ReaxFF MD) methods. In this seminar, two applications of CVD and ALD processes will be presented:

A. ReaxFF MD simulations were performed to clarify the effects of gas molecules on the reaction and growth mechanisms for silicon-germanium (SiGe) thin film using SiH_3 or SiH_2 and GeH_3 or GeH_2 in PECVD processes. Our results revealed that the film compositions could be estimated in these binary systems if gaseous species rations were identified because of the linear increase in Ge content in films. I proposed experimental setups and conditions, enabling the growth of high-quality films based on the results of ReaxFF MD simulations.
B. DFT and ReaxFF MD simulations were performed to clarify the effect of substrate temperature on the surface reaction and growth mechanism for boron nitride (BN) thin film using BCl_3 and NH_3 in the thermal ALD processes. The fundamental reaction mechanisms were analyzed by DFT simulations to develop a new force field for ReaxFF MD simulations. The four reactions were numerically analyzed and modeled in the force field: (a) BCl_3 reactions on OH-terminated Si(100) surface, (b) NH_3 reactions on Cl-terminated Si(100) surface, (c) BCl_3 reactions on H-terminated BN surface, and (d) NH_3 reactions on Cl-terminated BN surface. ReaxFF MD simulations were performed to grow BN thin films with continuous irradiations of BCl_3 and NH_3 molecules on the surface.

Chairs: Professors Yiming Li & Seiji Samukawa