Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Chemical Reactions and Atomic Removal Dynamics during Gallium Nitride Chemical Mechanical Polishing Process: Quantum Chemical Molecular Dynamics Simulations KENTARO KAWAGUCHI, YUJI HIGUCHI, NOBUKI OZAWA, MOMOJI KUBO, Fracture and Reliability Research Institute Graduate School of Engineering, Tohoku University — The chemical mechanical polishing (CMP) is promising for efficient polishing of the GaN substrate, and it is essential for manufacturing of GaN devices. However, the detailed CMP mechanisms are unclear, and then the design of efficient and precise CMP process is difficult. We performed polishing simulations of a GaN substrate by a SiO_2 abrasive grain in a solution including OH radicals in order to reveal effects of OH radicals on the polishing process. The OH radicals in the solution are adsorbed on the GaN surface and occupy the hollow sites on the surface. Then, a surface-adsorbed O atom is generated by the chemical reaction between the surface-adsorbed OH species and a OH radical in the solution. In the friction interface between the GaN substrate and the abrasive grain, the surface-adsorbed O atom is mechanically pushed into the GaN substrate by the abrasive grain. This O atom intrusion induces the dissociation of Ga-N bonds of the GaN substrate. Moreover, volatile N_2 molecules and soluble $Ga(OH)_3$ molecules are generated due to the dissociation of Ga-N bonds. Then, we suggested that the GaN CMP process efficiently proceeds by the mechanically induced chemical reactions: a surface-adsorbed O atom is generated and pushed into the GaN bulk by the abrasive grain.

Kentaro Kawaguchi
Fracture and Reliability Research Institute
Graduate School of Engineering, Tohoku University

Date submitted: 12 Nov 2014 Electronic form version 1.4