N2-P032

A Molecular Dynamics Study of the Stress Effect on Oxidation Behavior of Silicon Nanowires

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Silicon nanowires (Si NWs) have been extensively studied for nanoelectronics owing to their unique optical and electrical properties different from those of bulk silicon. For the development of Si NW devices, better understanding of oxidation behavior in Si NWs would be an important issue. For example, it is widely known that atomic scale roughness at the dielectric (SiOx)/channel (Si) interface can significantly affect the device performance in the nano-scale devices. However, the oxidation process at the atomic-scale is still unknown because of its complexity. In the present work, we investigated the oxidation behavior of Si NW in atomic scale by simulating the dry oxidation process using a reactive molecular dynamics simulation technique. We focused on the residual stress evolution during oxidation to understand the stress effect on oxidation behavior of Si NWs having two different diameters, 5 nm and 10 nm.

We calculated the charge distribution according to the oxidation time for 5 and 10 nm Si NWs. Judging from this data, it was observed that the surface oxide layer started to form before it is fully oxidized, i.e., the active diffusion of oxygen in the surface oxide layer. However, it is well-known that the oxide layer formation on the Si NWs results in a compressive stress on the surface which may retard the oxygen diffusion. We focused on the stress evolution of Si NWs during the oxidation process. Since the surface oxidation results in the volume expansion of the outer shell, it shows a compressive stress along the oxide layer. Interestingly, the stress for the 10 nm Si NW exhibits larger compressive stress than that of 5 nm Si NW. The difference of stress level between 5 an 10 anm Si NWs is approximately 1 or 2 GPa.

Consequently, the diameter of Si NWs could be a significant factor to determine the self-limiting oxidation behavior of Si NWs when the diameter was very small.

Keywords: Silicon, Oxidation, Molecular Dynamics