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Generation of core-shell structures and segregation of dopants in Si/SiO_2 nanowires SUNGHYUN KIM, JI-SANG PARK, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea — Oxidized Si nanowires (SiNWs) are usually synthesized by subsequent thermal annealing of as-grown SiNWs. It has been observed that B diffusivity is enhanced during thermal annealing in SiNWs, similar to the phenomena called transient enhanced diffusion or oxidation enhanced diffusion in planar Si/SiO_2 interfaces. However, previous theoretical studies have been focused on hydrogen or hydroxyl terminated SiNWs. In this work, we generate realistic atomic models for oxidized SiNWs in which crystalline Si core is sheathed by amorphous SiO_2 by using a combined approach of classical molecular dynamics simulations with first-principles density functional calculations. For realistic core-shell structures, we investigate the stability and segregation behavior of B and P dopants. A single substitutional B is more stable in the Si core, with a very small energy variation with the radial position of B. On the other hand, B dopants easily segregate to the oxide shell with the aid of Si self-interstitials generated during thermal oxidation. In contrast to B dopants, P dopants prefer to reside in the Si core even in the presence of Si self-interstitials but tend to aggregate in the Si region near the interface, forming nearest-neighbor donor pairs which are electrically inactive.

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