Simulation for SiC Power Electronic Device Developments

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Abstract

Silicon carbide (SiC), being a wide-band-gap semiconductor, is an attractive material in the development of electronic devices operated under extreme conditions such as high power, high temperature, and high radiation. SiC is particularly attractive for use in metal-oxide-semiconductor (MOS) technology because among the compound semiconductors only silicon carbide has the thermal oxide SiO₂, which is a good insulator. However, it is known that SiO₂/SiC interfaces have a higher density of interface traps than SiO₂/Si interfaces and that the channel mobility of MOS devices is much lower than theoretically expected values. In order to improve these characteristics, it is important to understand the thermal oxidation process at the SiO₂/SiC interface. In this report, we performed large-scale first-principles molecular dynamics simulations of the SiO₂/SiC interface oxidation process and the NO annealing. We also performed large-scale first-principles molecular dynamics simulations to generate amorphous SiO₂/SiC interface and calculated interface states using hybrid functionals.

KeyWords: First-principles molecular dynamics simulation, SiC power device, interface, thermal oxidation