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Boron diffusion mechanism and effect of interface Ge atoms in Si/SiO_2 and $SiGe/SiO_2$ interfaces GEUN-MYEONG KIM, YOUNG JUN OH, CHANG HWI LEE, K.J. CHANG, KAIST — In metal-oxide-semiconductor field effect transistors (MOSFETs) it is known that implanted B dopants easily segregate to the oxide during thermal annealing after ion implantation, causing threshold voltage shift and sheet resistance increase. On the other hand, SiGe alloys have been considered as a promising material for *p*-type MOSFETs due to reduced B diffusion and high hole mobility. However, there is a lack of studies for B diffusion in Si/SiO_2 and $SiGe/SiO_2$ interfaces. In this work, we perform first-principles density functional calculations to study the mechanism for the B diffusion in Si/SiO_2 and $SiGe/SiO_2$ interfaces. We investigate the diffusion pathways and migration barriers by using the climbing nudged elastic band and dimer methods. For Si/SiO_2 interface, B in Si turns into an interstitial B and tends to intervene between the Si and bridge O atoms at the interface. The overall migration barrier is calculated to be about 2 eV, comparable to that in bulk SiO_2. In $SiGe/SiO_2$, interface Ge atoms enhance the stability of B-related defects in the interface region, resulting in the higher migration barrier of about 3.7 eV. Our results indicate that Si/SiO_2 interface does not hinder the B diffusion, however, the B diffusion is suppressed in the presence of interface Ge atoms.

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