

Abstract Submitted
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Effect of Hydrogen on the Migration Processes of Dislocations in Silicon NORIHISA OYAMA, TAKAHISA OHNO, NIMS — It was reported that the dislocation glide mobility in Si is enhanced by irradiation with H plasma. In this work, we perform the first-principles total-energy calculations, and investigate the effect of H on the migration processes of dislocations in Si. We found that the most stable site in the dislocation core is not located at the bond center (BC) site but at the back-bond (BB) site. By interacting with a H atom, the formation energy of a kink becomes negative, and the dislocation is spontaneously bent. As a result, the activation energy of dislocation motion decreases by 1.1eV. The migration processes of the kinks are discussed in the presentation. This study was supported by RSS21 project and Grant-in -Aid for Scientific Research (No.17064017) of MEXT of the Japanese government. The calculations in this work were carried out partly using the Numerical Materials Simulator in National Institute for Materials Science (NIMS), and partly using the NEC-SX5 at Cybermedia Center, Osaka University.

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