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Kinetic Monte Carlo study for the thermal stability of hydrogen in ZnO JUNHYEOK BANG, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701 — Zinc oxide (ZnO) has attracted much attention due to a variety of applications to transparent optoelectronic devices. It is known that undoped ZnO exhibits n-type conductivity. Hydrogen, which is unintentionally incorporated, is considered as a promising candidate for shallow donors in ZnO. However, it is still difficult to explain n-type conductivity in annealed ZnO due to the low thermal stability of H. Here we study the diffusion of H in ZnO using first-principles calculations and then perform kinetic Monte Carlo (kMC) simulations for the thermal stability of H. The migration energy of a substitutional H is much higher than that for an interstitial H. Using as input the energy barriers for H diffusion, kMC simulations show that interstitial and substitutional H atoms diffuse out at different annealing temperatures around 125 and 475 ^{o}C, respectively, in good agreement with experiments. When H atoms are injected from air into ZnO, we find that they are likely to be trapped at O-vacancy sites, leading to the n-type conductivity in annealed samples.

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