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Thermal Stability of Hydrogen in ZnO Bulk and Thin Films: A Kinetic Monte Carlo Study

Authors : M. A. Lahmer, K. Guergouri

Abstract : In this work, Kinetic Monte Carlo (KMC) method was applied to study the thermal stability of hydrogen in ZnO bulk and thin films. Our simulation includes different possible events such as interstitial hydrogen (Hi) jumps, substitutional hydrogen (HO) formation and dissociation, oxygen and zinc vacancies jumps, hydrogen-VZn complexes formation and dissociation, HO-Hi complex formation and hydrogen molecule (H2) formation and dissociation. The obtained results show that the hidden hydrogen formed during thermal annealing or at room temperature is constituted of both hydrogen molecule and substitutional hydrogen. The ratio of this constituants depends on the initial defects concentration as well as the annealing temperature. For annealing temperature below 300°C hidden hydrogen was found to be constituted from both substitutional hydrogen and hydrogen molecule, however, for higher temperature it is composed essentially from HO defects only because H2 was found to be unstable. In the other side, our results show that the remaining hydrogen amount in sample during thermal annealing depend greatly on the oxygen vacancies in the material. H2 molecule was found to be stable for thermal annealing up to 200°C, VZnHn complexes are stable up to 350°C and HO was found to be stable up to 450°C.

Keywords : ZnO, hydrogen, thermal annealing, kinetic Monte Carlo
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