Nanostructured surfaces

DFT study of electronic and optical properties of ZnO thin films doped with In, Al and Ga

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Experimental studies [1] show that in ZnO:In films, with an increase in the indium dopant concentration from 1.7 to 6.6 wt.%, the optical bandgap width decreases from 3.30 to 3.27 eV due to the increase in the number of structural defects, the blue shift of the fundamental absorption edge in thin films of ZnO:Al and ZnO:Ga as the dopant level increases is due to the Burstein–Moss effect.

In the present work, we attempt to elucidate electronic structure and optical properties of In, Al and Ga-doped zinc oxide from the first-principles calculations using pseudopotential method, within density functional theory (DFT) with the Hubbard U corrections. To calculate various concentrations of doped atoms, a 2×2×2 supercell was constructed with 16 Zn and 16 O atoms. Electron-ion interactions were modeled using ultrasoft pseudopotentials in the Vanderbilt form. The wave functions of the valence electrons were expanded through a plane wave basis-set and accurate Brillouin zone integration was performed via careful sampling of k points chosen according to the Monkhorst-Pack scheme.

The calculated fundamental band gap and the lattice parameters of ZnO are close to the experimental ones and in a good agreement with other theoretical calculations. The calculated results show that the optical bandgap of In, Al, Ga-doped ZnO increase with an increase in dopant content, which leads to a blue shift of the optical edge absorption. The electronic structures show that the Fermi level of doped ZnO shift up to conduction band, which indicates obtaining of n-type ZnO with good electrical conductivity properties. The strong hybridization occurs between the 2p-O- and 5s-In (4s-Ga, 3s-Al) states at the Fermi level. These coupling levels mainly determine the optical properties of doped ZnO.

1. *Kapustianyk V. B., Turko B. I., Rudyk V. P., Kulyk B. Y., Rudko M. S.* Effect of dopants and surface morphology on the absorption edge of ZnO films doped with In, Al, and Ga// J Appl Spec.-2015.-**82**, N 1.-P. 153-156.