Quasi-Chemical Model of Point Defect Equilibrium in ZnO Single Crystal

Berestok T.O., Kosyak V.V., Kshnjakina S.I., Opanasyuk A.S.

Sumy State University, Sumy, Ukraine

Practical application of device structures based on single crystals and films of zinc oxide is determined by electro-physical and optical characteristics of the material, which is largely conditioned by the ensemble of point defects of the material. Point defects can be traps, luminescence and photoconductivity centers, act as donors and acceptors. Therefore, the ability to obtain semiconductors with controlled ensemble of point defects by varying the deposition condition determines the possibility of using the material.

In the work we report the results of improvement of modeling of the point defects equilibrium in zinc oxide single crystals, which is based on the consideration of the formation of point defects under thermodynamic equilibrium between gas phase and solid state [1].

The developed approach allowed us to obtain the balance of chemical potentials between perfect crystal and defect-containing crystals. On the basis of this approach we developed the equations that allowed more adequately calculations of the concentration of various types of point defects of zinc oxide during changing the external temperature of deposition or annealing.

Using obtained equations, translation, vibrational and rotational motions of the total defect energy were determined and estimation of the chemical potentials of the atoms of zinc (μ_{Zn}) and oxygen (μ_O) were made. As a result the dependence of the dominant point defect concentration and free charge carriers concentration on the growth conditions ZnO were studied. The values of the defects formation energy and transition energy levels calculated from the first-principles were taken from [2]. The concentration of free charge carriers and charged point defects were calculated using Fermi-Dirac statistics. On the basis of these values the concentration of point defects were expressed as a function of zinc and oxygen in the material by the values of the chemical potentials.

Moreover comparing analysis of results obtained by propounded model and traditional model of point defect ensemble modeling

1. Kosyak V., Mortazani Amiri N.B., Postnikov A.V., Scarpulla M.A. Model of native point defect equilibrium in Cu_2ZnSnS_4 and application to one-zone annealing // *Journal of Applied Physics*, **114**, (2013), 124501.
2. Zhang S.B., Wei S.-B., Zunger A. Intrinsic n-type versus p-type doping asymmetry and the defect physics of ZnO // *Physical Review B,* **63**, (2001), 07205.