The study of native defects and their interaction with donor Al impurity in ZnO by the help of fullerene like model

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We successfully used fullerene like (FL) cluster model earlier for a solution of band engineering problems in ZnO alloys and precipitation of CdO phase in these materials[1-5]. For the development the technology of growing and for the control of properties for ZnO based materials doped by Al and other impurities for the aim of applications in photovoltaic and optoelectronic devices, the minimization of donor impurities compensation by native acceptor defects (V_{Zn}, O_i etc.) is required. Exponential dependence of defect concentration on their formation energy results in the situation when almost only defects with minimal energy are present in any semiconducting material. For determination the thermodynamic properties of defects we started the series of computational experiments.

Qualitative results for the behavior of Al impurity in fullerene like cluster based on ZnO were obtained. Al impurity tends to uniform distribution in such clusters. Analysis of the defect formation energy shows the advantage in the formation of interstitial Oi in a comparison with a formation of Zn vacancy when Oi is adjacent to Al. Uniform distribution of Al impurity and nonadjacent position of Oi to Al increase Al ionization energy. Thus FLM demonstrated again its capability of living, what allows to use it in future for the control of the electroactivity of donor impurities of the third group due to their compensation by intrinsic acceptor defects of ZnO crystal lattice and to look for technological ways for improving the electroactivity of the donor impurity in ZnO. Adjacent position of Al atom to Oi decreases the energy of its formation and increases Al ionization energy. The results of theoretical calculations of Al ionization energy and adjacent V_{Zn} and O_i allowed us to formulate recommendations to the conditions of technological processes for ZnO films deposition.

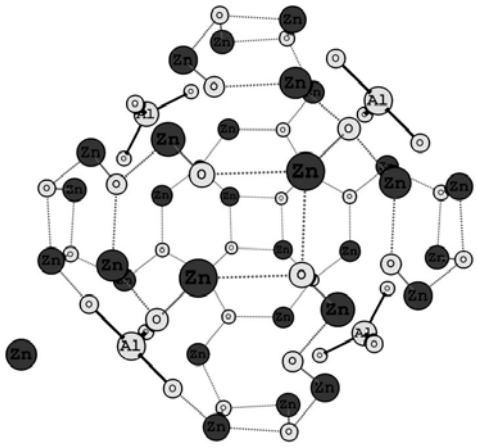

Fig.1. The geometry of the $Zn_{32}Al_4O_{36}$ cluster with Zn vacancy.

[1] L.I. Ovsiannikova, *Acta Physica Polonica A* **122**, 1062 (2012)..
[2] L.I. Ovsiannikova, *Acta Physica Polonica A* **126**, 1090 (2014)..
[3] L. Ovsiannikova, V. Kartuzov, I. Shtepliuk,G. Lashkarev, *Acta Physica Polonica A* **129**, A-41 (2016)..
[4] I.I. Shtepliuk, V. Khranovskyy , G. Lashkarev, et al., *Solid-State Electronics*, **81**, 72-77 (2013)
[5] L. Ovsiannikova, V. Kartuzov, G. Lashkarev, *45st "Jaszowiec" International Scool & Conference on the Physics of Semiconductors, Szczyrk, Poland, 2016*