The investigation of the cadmium effect on properties of ZnCdO alloys using $Zn_{36-x}Cd_xO_{36}$ clusters

L. Ovsiannikova, G. Lashkarev, V. Kartuzov and I. Shtepliuk

Frantsevich Institute for Problems of Material Science, NASU, 03680, Kiev-142, Ukraine, Phone +38 044 4240102, avilon57@ukr.net

Using the models of atomic clusters for the solution of problem of band-gap engineering of nanomaterials based on ZnO was proposed. Previously the dependences of electronic structure of Zn_nO_n and $Zn_{n-x}Cd_xO_n$ fullerene-like and wurtzitic-like clusters on the amount of atoms in cluster and their geometry were investigated. The model of $Zn_{60}O_{60}$ fullerene-like cluster with the shell of diamond-like structure and sp^2/sp^3 type of bonds has been constructed. [1, 2].

Model of the fullerene-like $Zn_{36-x}Cd_xO_{36}$ cluster with sp^2 bonds was proposed for investigations of the influence of the cadmium impurity in the ZnO matrix on the geometric structure, cohesive properties, electronic structure and band-gap width of ZnCdO ternary alloys (Fig. 1). The optimized geometry, total energy and band-gap width of the clusters were determined within the B3LYP electron density hybrid functional method with 3-21G(d) basis sets. The cohesive energy was computed as a difference between the total energy of the cluster and the total energy of noninteracting constituent atoms.

Calculations for clusters with Cd content of 5.5, 11, 16.7, 22 and 33% are presented. It was shown that a substitution of Zn atoms by Cd ones leads to changing of bond lengths, valence angles, redistribution of ions charges and, consequently, gives rise to the reduction of the cluster stability with an increase of Cd content. The monotonical decrease of the energy gap with an enlargement of the Cd content was also revealed (Fig. 2). In our previous work we have investigated the electrical and optical properties of the n-$Zn_{0.94}Cd_{0.06}O$/p-SiC heterostructures, which exhibited reasonable rectification behavior and diode characteristics [3]. It was revealed that the calculated band-gap energy (2.827 eV) for $Zn_{34}Cd_2O_{36}$ cluster (~6 at.% Cd) is very close to the experimental value of the band-gap (2.87 eV) for $Zn_{0.94}Cd_{0.06}O$ films grown by rf magnetron sputtering technique.

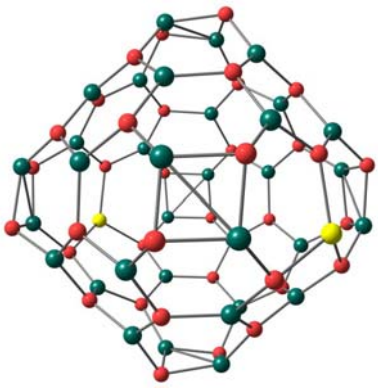

Fig.1

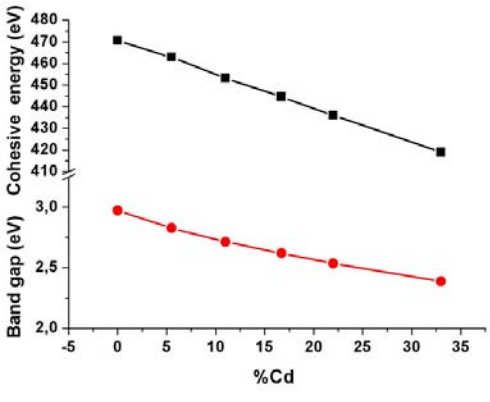

Fig.2

Fig.1. The optimized geometry of the $Zn_{34}Cd_2O_{36}$ cluster (~6 at.% Cd); ● light balls – Cd.
Fig.2. The dependence of cohesive energy and band-gap width on Cd content in the cluster.

[1] L.I. Ovsiannikova, *Acta Physica Polonica A* **122**, 1062 (2012).
[2] L.I. Ovsiannikova, *Acta Physica Polonica A* **124**, 862 (2013).
[3] I.I. Shtepliuk, V. Khranovskyy , G. Lashkarev, V. Khomyak, V. Lazorenko, A. Ievtushenko, M. Syvajarvi, V. Jokubavicius, R. Yakimova, *Solid-State Electronics,* **81**, 72 (2013).