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**ELECTRONIC PROPERTIES OF DOPED ZnO FILMS:  
AB INITIO CALCULATIONS**
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 PACS 73.20.At  
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A change of the electron density distribution and a transformation of energy states of ZnO films with various thicknesses and different impurities (Cu, C, and Ag atoms) are investigated. The effects of compression, hydrogenization, and a defect of the number of atoms on the surface are examined. The results were obtained in the frame of the theory of pseudopotential by *ab initio* calculations and with the use of the electron density functional.

**1. Introduction and Statement of the Problem**

Thin films of ZnO are intensively studied in the last years, because this material has a wide range of applications in technology. Oxide ZnO is the well-known, chemically and thermally stable semiconductor of the *n*-type which is sensitive to toxic and flammable gases. Pure and doped films of ZnO are studied as a basis for sensors of O<sub>2</sub> [1], H<sub>2</sub> [2], NO<sub>x</sub> [3], ethanol [4], CO, CH<sub>4</sub> [5], *etc.* Pure oxide ZnO and one with Cu atoms on the surface are used as catalysts in chemical reactions [6]. Oxide ZnO with impurities Ga and In is a very sensitive inorganic scintillator and is useful in the registration of alpha-particles [7]. Due to the wide energy gap (3.32 eV), semiconductor ZnO is attractive for the designers of light diodes/lasers which emit light with small wavelengths and is used as a material for transparent conducting films. As a nanomaterial, ZnO is realized in various morphological forms: nanofilms, nanowires, nanorods, and nanospheres [8–19]. Recently, the possibility to use nanorods in short-wave lasers was demonstrated in [20–22]. For all mentioned applications of ZnO, of special meaning are the data on its behavior on the nanoscale.

Zincite (ZnO) is crystallized into a structure of the wurtzite type with the following parameters of an elementary cell:  $a = b = 3.249 \text{ \AA}$ ,  $c = 5.205 \text{ \AA}$ . Oxygen

atoms O form a two-layer dense packing, where zinc Zn occupies a half of tetrahedral voids of a single orientation. In its structure, the layers of various atoms alternate along the crystallographic axis  $\bar{c}$  and cause the polarity of crystals: Zn<sup>2+</sup> and O<sup>2-</sup> form layers (0001) and (000 $\bar{1}$ ), respectively. The distances Zn–O along the axis  $\bar{c}$  are 1.992 Å and are equal to 1.973 Å along two other directions. In the hexagonal structure of wurtzite, each anion is surrounded by 4 cations which are placed at the vertices of a tetrahedron (the same is true for cations). It is a typical coordination  $sp^3$  of the covalent bonding, but ZnO has also a significant ionic character (a degree of ionicity equals 0.675). The electron configurations of O and Zn are, respectively:  $1s^2 2s^2 2p^4$  and  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$ . Orbits  $2s$  and  $2p$  of atoms form the occupied valence band, levels  $4s$  of Zn<sup>2+</sup> for the conduction band, and levels  $3d$  of Zn are hybridized with levels  $2p$  of O according to the tetrahedral symmetry and are responsible for the covalent component of the bonding of ZnO. A wurtzite crystal is bounded by the surfaces (1010) and (1120) which are nonpolar and by the polar ones, (0001) (Zn) and (000 $\bar{1}$ ) (O) (Fig. 1) [23, 24]. By the ionic deposition with a subsequent annealing at not too high temperatures, all four types of surfaces with the arrangement of atoms like that in bulk can be obtained.

The analysis of polar surfaces meets the fundamental problem which is due to the ionic model of those surfaces, according to which they are unstable and cannot exist. They are named the Tasker surfaces of type 3 [25]. Using the simple arguments of electrostatics, it can be shown that the surface energy diverges for such a configuration of ions. However, the polar surfaces of ZnO are amusingly stable in reality, and many experiments demonstrate that they exist in the nonreconstructed, pure, and

completely ordered state [26]. Despite the significant number of studies, the question about the mechanisms of stability of polar surfaces of ZnO remains unanswered. For example, the authors of work [27] performed *ab initio* calculations and considered that the stabilization of polar surfaces is attained by the transport of charge as a result of the strong compression of double layers Zn–O. Such a compression from 20% to 50% was observed in some experiments [28, 29, 30]. Other researchers [31, 32, 33] conclude, on the contrary, that the distance between Zn–O layers is the same as in bulk. Recently, a new mechanism of stabilization of the surface of Zn atoms was proposed in [34], where the authors used the scanning tunnel microscopy and observed a deficit of about 25% atoms of Zn on the surface. Possibly, such a reduction in the number of Zn atoms on the surface is sufficient for the transfer of the charge necessary for its stabilization. Another possible mechanism of stabilization of the O surface by means of the covering of it by hydrogen, whose concentration was not reliably determined, was observed in experiments on the scattering of helium [35]. Thus, the data on the atomic and electronic reconstructions, as well as energies and the dispersion width of states related to the broken bonds of ions of polar surfaces in ZnO, are contradictory. Therefore, the additional information for their clarification is urgently needed. Another problem restricting the development and the application of ZnO-based optoelectronic devices is related to the absence of  $p-n$  junctions in ZnO. It is known that as-produced ZnO is a semiconductor of the  $n$ -type with many donor defects such as  $V_O$  and  $Zn_i$ . Therefore, it is very difficult to dope ZnO in order to make it a semiconductor of the  $p$ -type due to the self-compensation by donor defects. Oxide ZnO was doped by elements of the I-st and V-th groups with positive results. The alloying by C (element of the IV-th group) was mainly studied in the context of magnetic properties [36,37], whereas its effect on the  $p$ -transformation was examined superficially [38,39]. The influence of the defects  $C_{Zn}+O_i$  on the transition of films of ZnO to the  $p$ -type was considered in [38]. *Ab initio* calculations made in [39] indicate the possibility of the  $p$ -transformation if C replaces O at a concentration of 12.5%. In this case, the acceptor level was by 0.33 eV above the top of the valence band. The authors of works [40, 41] assumed that the alloying of ZnO by Cu atoms should be accompanied by the appearance of holes. For example, Cu has the electron configuration  $3d^94s^2$  and reveals the tendency to form ion  $Cu^{1+}$  with the electron configuration  $3d^{10}4s^0$  and an ion radius of 0.6 Å which is close to the radius of  $Zn^{2+}$ . This allows one to consider that the

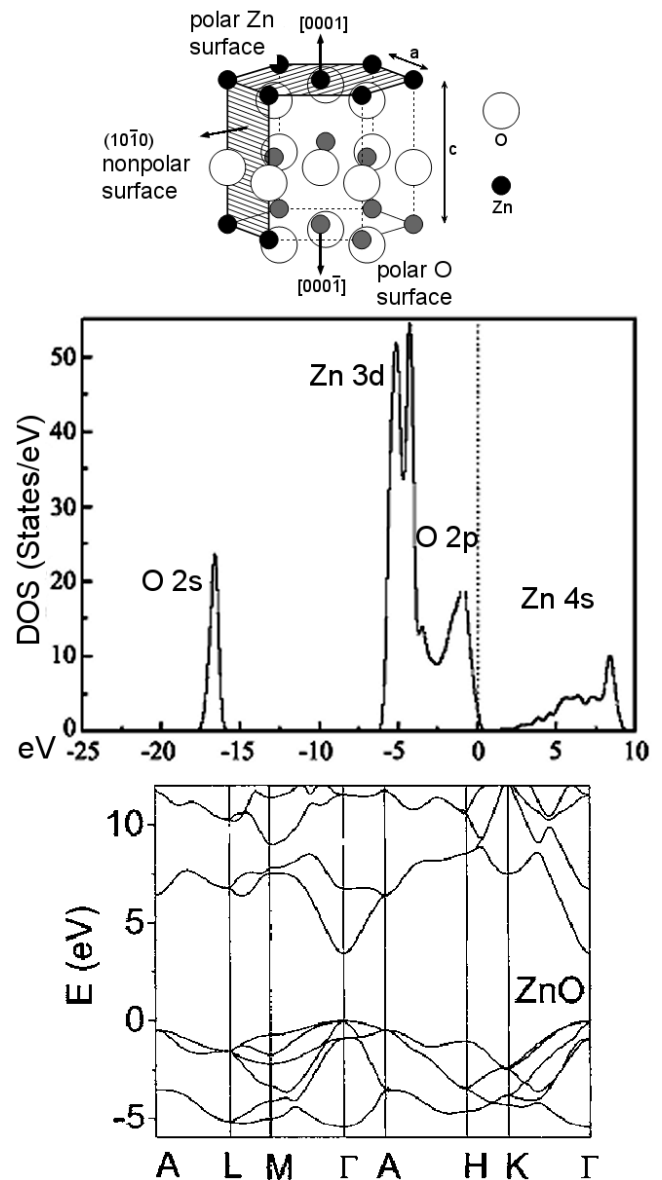


Fig. 1. Atomic structure, the density of states, and the band structure of bulk ZnO [23, 24]

replacement of Zn by Cu atoms will lead to the configuration of  $Cu^{1+}$  with an associated hole. Atom Li has the electron configuration  $1s^22s^1$  and, like Cu, try to form a single-charge cation ( $1s^22s^0$ ) with an ion radius of 0.59 Å which is close to the radius of  $Zn^{2+}$ , and can be also a supplier of holes [42]. However, the mechanisms of interaction of ZnO with impurities are studied else slightly.

In the frame of the present work with the use of the electron density functional and the pseudopotential, we

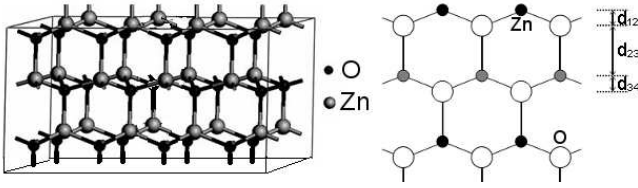


Fig. 2. Elementary cell of a film of ZnO made of 6 atomic layers and the cross-section perpendicular to the surface; the distances between layers are denoted

carry out *ab initio* calculations to examine a redistribution of the electron density and a transformation of energy states in thin films of ZnO doped by atoms Ag, C, or Cu. The comparison with pure films is performed to clarify the transformation of the type of conduction of ZnO to the *p*-type. The films have 4 or 6 atomic layers in thickness and polar surfaces. The effects of compression, hydrogenization of the surface of films, and a defect of the number of atoms on the surface are examined with the purpose to comprehend the nature of the stabilization of polar surfaces.

## 2. Models and Methods of Calculation

The results were obtained with the help of the authors' program code [43] which realizes the Car–Parrinello quantum-mechanical dynamics with the use of a local approximation in the formalism of the electron density functional [44, 45] and an *ab initio* norm-conserving pseudopotential [46]. The ground states of electron-nucleus systems were determined by the algorithm of quantum dynamics if variables of the electron and nuclear subsystems are simultaneously optimized or by means of the diagonalization of the Kohn–Sham matrix of a system if only the electron variables are determined at fixed atomic cores. Following works [47, 48], we write the electron density in terms of occupied orthonormalized one-particle wave functions:

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2. \quad (1)$$

In the Born–Oppenheimer approximation, a point on the potential energy surface was determined by a minimum with respect to the wave functions of the energy functional:

$$E[\{\psi_i\}, \{R_j\}, \{\alpha_\nu\}] = \sum_i \int_{\Omega} d^3r \psi_i^*(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 \right] \times \psi_i(\mathbf{r}) + U[\{n(\mathbf{r})\}, \{R_j\}, \{\alpha_\nu\}], \quad (2)$$

where  $\{R_j\}$  are the coordinates of nuclei, and  $\{\alpha_\nu\}$  stands for all possible external influences on the system.

In the commonly accepted approach, the minimization of an energy functional with respect to one-particle orbitals  $\psi_i$  under additional conditions of orthonormalization imposed on  $\psi_i$  leads to the Kohn–Sham self-consistent one-particle equations:

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + \frac{\delta U}{\delta n(\mathbf{r})} \right\} \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r}). \quad (3)$$

We expand the one-particle wave function  $\psi_i$  in a series in plane waves. The series length was chosen to be such that about 20 plane waves correspond to one atom (the number of waves was limited by the power of a computer). In the case where only the electron variables were sought at fixed cores, we calculated the Kohn–Sham matrix for Eq. (3) at a certain value of the wave vector  $\mathbf{k}$  from the Brillouin zone. The matrix is composed from elements on the operators of kinetic energy and the ion pseudopotential which is screened by the dielectric function  $\epsilon(\mathbf{G})$  in the Thomas–Fermi approximation:

$$\epsilon(\mathbf{G}) = 1 + \frac{3}{2} \frac{4\pi z e^2}{\Omega G^2 E_f^0}. \quad (4)$$

Here,  $E_f^0 = \left( 3\pi^2 \frac{z}{\Omega} \right)^{2/3}$  is the Fermi energy of a free electron gas, and  $z$  is the number of electrons in volume  $\Omega$ .

The diagonalization of the Kohn–Sham matrix allows us to obtain coefficients in the expansions of the wave function and the energy spectrum  $E_i(\mathbf{k})$ .

To reproduce a film of ZnO which is infinite in two directions and has two polar surfaces (0001) (Zn) and (000 $\bar{1}$ ) (O), we constructed the atomic basis of a primitive tetragonal cell of the superlattice which is composed of 32 atoms and includes 4 atomic layers or of 48 atoms and includes 6 atomic layers (Fig. 2). The size of the elementary cell which reproduces the translational symmetry of the system of atoms was taken  $4 \times 1$  (as compared with the size of a wurtzite cell of  $1 \times 1$ ) in a plane which is parallel to the surface. This allowed us to create a quite significant concentration of impurities. In a plane perpendicular to the surface, the size was chosen such that the translationally repeated films do not influence one another.

The calculations were performed only for the  $\Gamma$ -point of the Brillouin zone of the superlattice in view of the fact that just it is referred to the fundamental energy gap of a ZnO crystal and, as shown in all known studies, does not change its position, when the morphology of ZnO

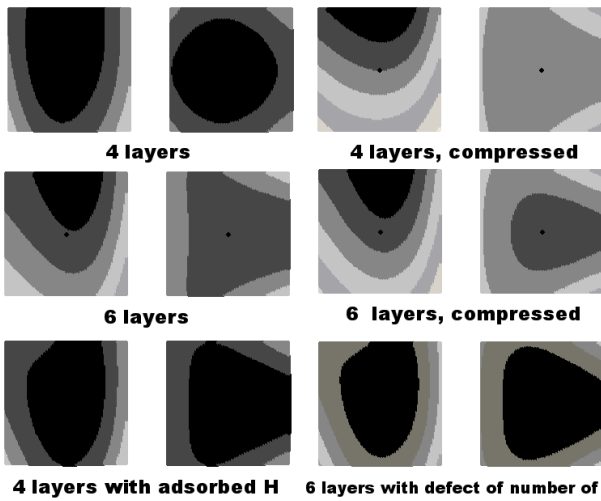


Fig. 3. Section of the bulk electron density in the neighborhood of Zn atom from the surface layer (0001) in various models which were calculated

varies at the transition to the nanoscale. The number of valence electrons for Zn was taken 12 with regard for 10  $d$ -electrons of the previous shell. That is, the electron configurations of ionic cores within the pseudopotential ideology were considered  $3d^{10}4s^2$  for Zn and  $2s^22p^4$  for O, respectively.

### 3. Results of Calculations and Their Discussion

We do not optimize the atomic basis of a supercell. To clarify the mechanisms of stabilization of the polar surface of a ZnO film, we carried out calculations for 4- and 6-layer films without compression of Zn–O layers with pure surfaces and with the arrangement of atoms like that in bulk; for a 6-layer film with the compression of layers to their positions which were obtained in [27]: distances  $d_{23}$  between the external layers (see Fig. 2) were reduced by 50% relative to the bulk ones; for a 4-layer noncompressed film, for which the surface with O was covered by atoms of hydrogen placed on the positions of the next layer at the distance of a hydroxyl group; and for a 6-layer noncompressed film with a defect of the number of atoms Zn on the surface at a concentration of 25%. We determined the distributions of the electron density in bulk and on the surface of a film (Fig. 3) and the density of states for the  $\Gamma$ -point of the Brillouin zone.

It is known that the compression of a film can change its structure of the wurtzite type to that of rock salt [49]. As indicated in [27], such a change occurs at pressures more than 9 GPa. But, at the compressions attained in the present work, the pressure was lower (the calculation

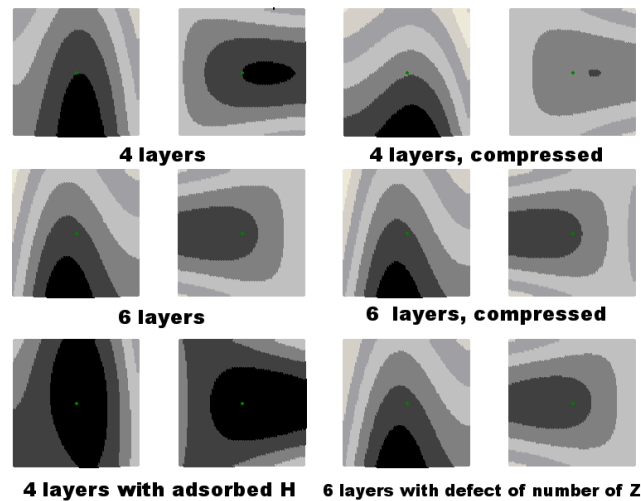


Fig. 4. Section of the bulk electron density in the neighborhood of O atom from the surface layer (000 $\bar{1}$ ) in various models which were calculated

pressure was at most 7 GPa). Hence, we consider that the film structure is invariable.

By analyzing the changes of the distributions of valence electrons in the region of surfaces, we can evaluate the extent of the influence of the internal electric field on the total distribution of the electron density. First, it is seen that an increase in the film thickness causes a decrease in the charge of surface atoms on both bounding surfaces. This fact allows us to conclude about a decrease in the influence of the electric field arising between polar surfaces, as the thickness of films increases, in agreement with results in [27]. A similar outflow of the electron charge is observed for compressed films with various thicknesses. Moreover, this is more pronounced for thin films. Other, but similar to one another, patterns of a transformation of the charge on surfaces are observed for films with adsorbed hydrogen on a surface of O and with a defect of the number of Zn atoms on the Zn surface up to 25%. Here, on the contrary, the charge inflow to surface atoms is observed.

As for the energy gain in various models of a film, the atomic configurations lowest in energy are observed in thicker films, where the stabilization of surfaces can occur due to a compression of layers or due to the adsorption of hydrogen. The energies of such atomic configurations are close, whereas the configurations with broken stoichiometry have higher energies.

As for the clarification of the transformation of the conduction type of ZnO to the  $p$ -type, we carried out calculations for 6-layer noncompressed film, for which a part of atoms of zinc or oxygen was replaced by other

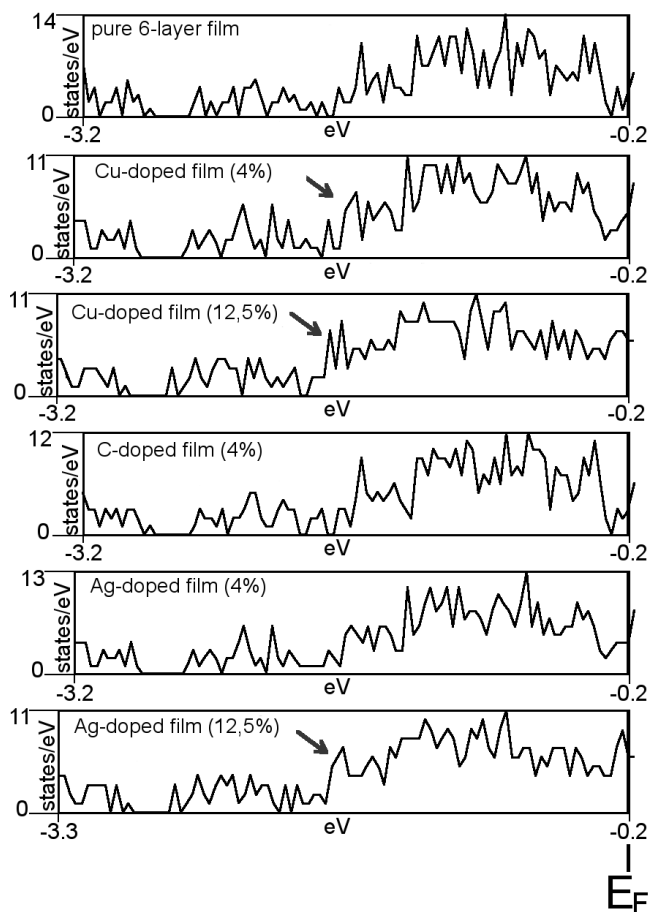


Fig. 5. Distribution of electrons over energy bands for the  $\Gamma$ -point of the Brillouin zone. The vertical axis gives the number of states, and the horizontal axis represents the energy range

atoms. In Fig. 5, we present the distribution of electrons over energy bands for the  $\Gamma$ -state. This distribution was obtained by numerical calculations of the derivative  $\lim_{\Delta E \rightarrow 0} \frac{\Delta N}{\Delta E}$ , where  $\Delta N$  is the number of allowed states which fall in the energy interval  $\Delta E$  of a one-particle energy spectrum  $E_i(k=0)$  obtained in the course of the diagonalization of the Kohn–Sham matrix. The number of energies in the spectrum was controlled by the size of the expansion of a wave function. According to the ideology of the electron density functional, we determined the occupied states at  $T = 0K$ , which allowed us to find a position of the Fermi level with regard for the last occupied state. The number of occupied states was determined by the half-number of electrons (because the spin of electrons was not considered). The information about the following unoccupied allowed state gives us a possibility to determine the position of the first unoccu-

ried state (the bottom of the conduction band) and the presence of the energy gap.

The comparison of the calculated distributions of states of valence electrons for the  $\Gamma$ -point of a ZnO film with two surfaces of dangling bonds with an analogous distribution for bulk ZnO is complicated by the presence of additional states due to surface atoms and impurity atoms. Therefore, the obtained distributions were used only for relative comparisons at a change of the chemical composition of the film.

The analysis of the density of states for the  $\Gamma$ -point of the Brillouin zone (Fig. 5) indicates that the valence band extends at the replacement of Zn atoms by atoms of copper and silver at concentrations of 4% and 12.5%, respectively, which is related to the hybridization of states. In addition, we see, in all the cases, the formation of new energy levels in the lower part of the valence band, which is related to  $2p$  states of O and  $3d$  states of Zn (Cu or Ag) (see arrows in Fig. 5). In this case, the formation of such levels is less pronounced for silver. As for the introduction of carbon at a concentration of 4% into positions of oxygen, no considerable changes in the structure of the energy spectrum were observed, as distinct from the conclusions drawn in [39] at a carbon concentration of 12.5%.

#### 4. Conclusions

1. Within the methods of electron density functional and pseudopotential with *ab initio* calculations, we have obtained the distributions of the density of valence electrons and the electron energy spectra for thin ZnO films doped with Ag, C, or Cu atoms at concentrations of 4% and 12.5%. The thickness of films was 4 or 6 atomic layers. The effects of compression, hydrogenization of surfaces, and a defect of the number of atoms on the surface are examined.
2. The stabilization of polar surfaces of a ZnO film is realized due to a redistribution of the density of valence electrons.
3. An increase in the thickness of a ZnO film causes a decrease in the charge related to surface atoms on both bounding surfaces. A similar outflow of the electron charge is observed at a compression of thin films.
4. Another type of the charge transformation, namely the inflow of charge to surface atoms, is observed for ZnO films with hydrogen absorbed on the O surface and with a defect of the number of Zn atoms up to 25% on the Zn surface.
5. At the replacement of Zn atoms in a film of ZnO by atoms of copper and silver at concentrations of 4% and

12.5%, respectively, we have observed a spreading of the valence band, which is related to the hybridization of states. In this case, the new energy levels are formed in the lower part of the valence band which are related to  $2p$  states of O and  $3d$  states of Zn (Cu or Ag).

6. Introduction of carbon at a concentration of 4% into positions of oxygen gave no considerable changes in the structure of the energy spectrum of valence electrons.

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Received 04.09.09.

Translated from Ukrainian by V.V. Kukhtin

#### ЕЛЕКТРОННІ ВЛАСТИВОСТІ ЛЕГОВАНИХ ПЛІВОК ZnO: РОЗРАХУНОК ІЗ ПЕРШИХ ПРИНЦИПІВ

*Р.М. Балабай, П.В. Мерзликін*

#### Резюме

Досліджено зміну розподілу електронної густини та трансформацію енергетичних станів у плівках ZnO різної товщини та з різними домішками (Cu, C, Ag) при стисканні плівки та без нього, з гідрогенізацією поверхні плівки або з введенням дефекту кількості атомів на поверхні. Результати одержано в рамках теорії псевдопотенціалу із перших принципів та функціоналу електронної густини.