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# ABOUT FLUCTUATIONS OF THE BAND GAP OF POLYCRYSTALLINE MIXED FILMS $ZN_XCU_{1-X}O$

M.E. Kumekov

Taraz State University named after M.-Kh.Dulati, Taraz, Kazakhstan, kumekov@ntu.kz

*It is shown that fluctuations of the band gap caused by fluctuations of thickness of a film ΔL at presence of dimensional quantization of the energetic spectra of electrons and holes can satisfactory explain the change of width of the forbidden band observable experimentally in mixed films* $Zn_XCu_{1-X}O$.

**Keywords:** dimensional quantization, forbidden band, fluctuations, energy spectra, mixed film.

In work [1] results of measurements optical transmission of mixed films copper and zinc oxides are presented.

In the present work results of measurements optical transmission films of copper and zinc oxides are explained by the dimensional quantization of energetic spectra of the electrons near to bottom of a band of conductivity and to top of a valence band.

Film CuO with the best optical and electric properties turned out jet magnetron dispersion of a copper target then amorphous metal a film were oxidized in an atmosphere up to condition CuO (by means of heating at 500°C).

Relatives on quality were also a film, received cathodic dispersion of copper and the subsequent heating of the films in an atmosphere. Evaporation of a film by this method occurred to smaller speed, however partial pressure of argon was greater $10^{-2}$-$10^{-3}$ Torr, therefore a film of copper oxide received by the given method were practically identical to the films received with use magnetronic dispersions.

Investigated oxide films [2] were made by means of magnetronic evaporation of metals on glass substrates and the subsequent them heating in an atmosphere. For introduction of copper in structure of a film, a part of a zinc target became covered by copper. Thermal oxidation in an atmosphere was spent within an hour at $500^0$C.

The manufacturing techniques of films did not allow creating a film with absolutely homogeneous thickness so at average thickness of a film of roughness of 100 nanometers on thickness could make up to 10%.

In figure 1 the spectra of transmission are presented: a film copper oxide (1), a film received at 50 % covering Zn of a target the copper (2), not alloyed film zinc oxide on a substrate n - type (3), and a glass substrate (4).

Considering, that to value of band gap CuO there corresponds energy of quantum of light of an infra-red range, has been carried out also research optical transmission the films CuO and mixed films Cu (Zn) O in infra red (IR) areas.

In figure 2 spectra of transmission the films in infra-red light are represented. Spectra: 1-glass substrate, 2-ZnO, 3 Cu (Zn95 %) O, 4 - Cu (Zn75 %) O, 5 - Cu (Zn63 %) O, 6-CuO.

From comparison of spectra it is visible, that at greater concentration Cu in a film the sharp increase in absorption is observed at энергиях quantum of light, greater 0.8 эВ, it is connected with presence of phase CuO in these films. From figures strong degradation of edge of own absorption CuO in the red party up to 0,8eV is visible. The effective forbidden band decreases from the values 1,45 eV for monocrystals up to 0,8eV for investigated films. Similar degradation of edge of fundamental absorption of the copper oxide was observed in work [3] for nanopowders and nanoceramics. Authors of the given work connect reduction of effective width of the forbidden band for nanopowders and nanoceramics CuO with occurrence of intra slot levels with high density of states in nanooxides 3d - metals.

Since electronic structure CuO is characterized by strong electronic correlations already at the sizes of polycrystallites less than 50 nanometers start to be shown red shift of edge of absorption in CuO.

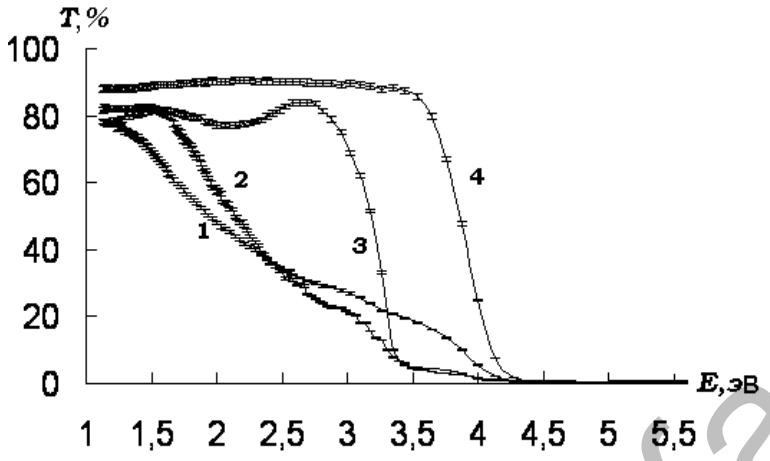


Fig. 1. The spectra of transmission of the different films (see text)

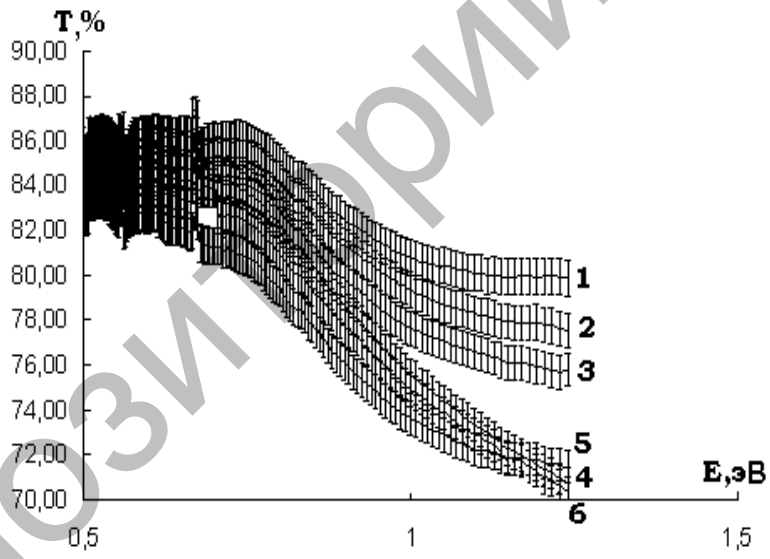


Fig. 2. The spectra of transmission of the different films in infra-red region

Polycrystalline mixed film are in the certain sense analogue of the disorder systems, intermediate between an ideal crystal and the amorphous environment. Fluctuations of the sizes of polycrystallite of a different phase cause change of the important properties, in particular, reorganization of a energetic spectrum, degradation of edge of a zone of conductivity and a ceiling of a valence zone, occurrence of tails of density of states in the forbidden band.

Let's consider the mechanism of change of edge of a zone (between valence band Ev and band of conductivity $E_C$), the zero energy of dimensional quantization connected with fluctuations in films with non-uniform thickness. For the account of influence of fluctuations of the sizes polycrystalline granule of the different phase we use the model within the limits of quantum dimensional effect. We shall consider that polycrystalline structure represents a thin film of average thickness L.

Fluctuations of thickness of the films make ΔL. The maximal thickness is equal L + ΔL, and minimal L- ΔL. Shift of edge of a zone can be counted as size of zero energy of the dimensional quantization corresponding with the first level.

As is known, (see, for example [4]) zero-point energy of dimensional quantization is defined as

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}. \quad (1)$$

Here m - effective mass of the carrier of a charge.

From (1) follows, that the fluctuations of zero-point energy connected with fluctuations of thickness пленок ΔL, will be equal:

$$\Delta E_1 = \frac{\pi^2 \hbar^2 \Delta L}{mL^3} \quad (2)$$

Change of the band gap $\Delta E_g$ is connected with shift of edges of a band of conductivity and a valence band. Then from (2) follows:

$$\Delta E_g = \Delta E_c + \Delta E_v = \frac{\pi^2 \hbar^2 \Delta L}{L^3}\left(m_c^{-1} + m_v^{-1}\right). \quad (3)$$

Here $m_c$ and $m_v$ are electrons and holes effective masses respectively.

In view of absence in the literature of unequivocal values of effective masses we shall result received of (3) through estimates for fluctuations of width of the forbidden band $\Delta E_g$ of CuO ($m_c$ =0,02 $m_0$ and $m_v$ =0,5 $m_0$):

$$\Delta E_g = 32{,}5\ (\Delta L/L)\ \text{eV}. \quad (4)$$

From (4) follows that already at average thickness of film L=100 nanometer the ratio of the attitude ΔL/L equal 0,01, $\Delta E_g$ becomes equal 0,325 eV.

This value of fluctuation $\Delta E_g$ can be quite used for an explanation of the change of width of the forbidden band observable experimentally on the films of the copper oxide and mixed films, caused by fluctuations of thickness of a film ΔL.

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