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ABOUT THE MECHANISM OF THE FORMATION OF POLYCRYSTALLINE HETEROJUNCTION n-ZnO/p-CuO

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On the basis of the analysis of crystalloid structure of copper and zinc oxides and for double charged Cu^{++} u Zn^{++} ions radiuses it is shown the possibility of the formation of the heterojunction between crystalline oxides of copper and zinc.

Keywords: crystalloid structure, heterojunction, crystalline oxides, cubic syngonies.

As is known [1] the formation of the heterojunction demanding joining of crystal lattices is possible only at concurrence of type, orientation and the period of crystal lattices both materials. These conditions define epitaxial attitudes for the fabrication of the heterojunction in cases of two various materials with identical crystal structure. Epitaxy is easily carried out, if the difference of parameters of both lattices does not exceed 10 % [2]. Under these conditions the heterojunction is formed in the mono crystal block.

Most often for the fabrication of the heterojunction use the substances with cubic syngonies, having close values of a constant lattice. In figure 1 the dependence of the band gap of typical semiconductors with the structures of diamond and zinc-blende on constant lattice used for the fabrication of the heterojunctions [3] is resulted.

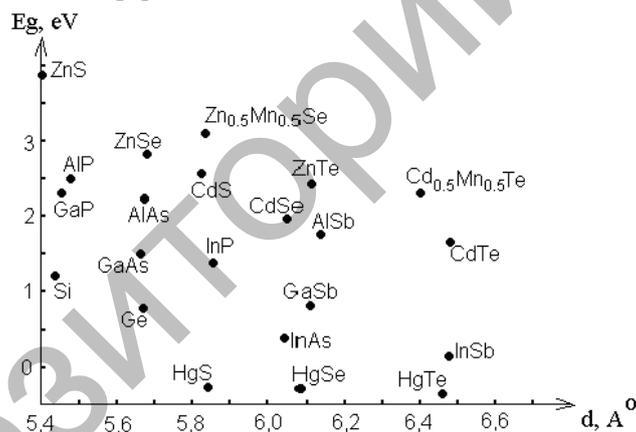


Fig. 1. Constants of lattices and width of the forbidden band for substances with cubic singony [3]

As angles between sides in cubic system are identical that, knowing values of a constant lattice, it is possible to do assumptions of an opportunity of creation of the heterojunction on investigated substances with a cubic lattice.

Studying opportunities of escalating of the heterojunctions in systems with different syngonies we have come to conclusion [4, 5], that for indissoluble continuation of a lattice of one substance by another, basically enough that even on one of sides of each lattice had close geometrical parameters. Technologically the formation of the heterojunction from materials with different syngonies is possible consecutive evaporation of the films of two different materials and their subsequent crystallization by a heating's method.

The processes occurring at such technique of formation of the heterojunctions, are complicated and diverse. This processes include formation crystalline structures of system grain – inter granular border - a germ. Growth of germs, and sometimes and their formation are facilitated, if between a germ, one of grains and inter granular border exist epitaxial attitudes [6]. Thus, crystallization on

inter granular borders according to a necessary minimum of energy will occur in the places satisfying to epitaxial attitudes.

According to radiographic measurements on the films ZnO and CuO, lead in [4, 5], parameters of crystal lattices can be tabulated.

Table 1

Substance	ZnO	CuO
Syngony	wurtzite	monoclinic
Basic vector a	$a=3.2489 \text{ \AA}$	$a=4.684 \text{ \AA}$
Basic vector b	$b=3,249 \text{ \AA}$	$b=3,425 \text{ \AA}$
Basic vector c	$c=5,206 \text{ \AA}$	$c=5,129 \text{ \AA}$
Angle between ribs b and c , a and c	$\alpha=\beta=90^\circ$	$\alpha=\beta=90^\circ$
Angle between b and a	$\gamma=120^\circ$	$\gamma=99^\circ 28'$

Apparently from the table, epitaxial attitudes are carried out for sides, constructed by vectors **b** and **c** and with angles $\alpha=\beta=90^\circ$ (see figure 2).

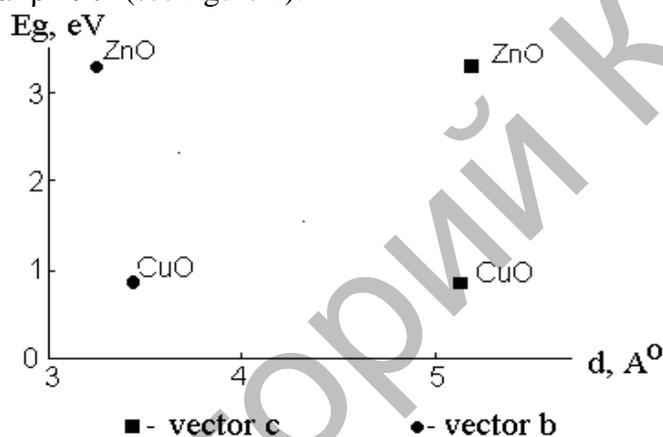


Fig. 2. Constants of lattices and width of the forbidden band for ZnO and CuO

Change of a chemical compound is known, that at formation of the heterojunction between semiconducting materials of type $A_{III}B_V$ and their firm solutions on the basis of arsenide's, phosphides and antimonides. Ga and Al occurs without change of the period of a lattice owing to affinity covalent radiuses Ga and Al. Ionic radiuses double charged ions Cu^{++} and Zn^{++} make close values: $0,8 \text{ \AA}$ and $0,83 \text{ \AA}$ accordingly [7]. Therefore the formation of the heterojunction in system ZnO / CuO on the planes of the sides with vectors **b** and **c** also does not lead to change of the period of a hetero lattice.

Thus, in this work on the basis of the analysis of crystal structure and values of ionic radiuses the opportunity of formation polycrystalline heterojunction in system ZnO / CuO is shown.

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