

## Theoretical Analysis of Nanostructure of Chalcogenide Amorphous Films

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It was found that thin chalcogenide films  $A^I\text{-Bi-C}^{VI}$  ( $A^I$  – Li, K, Na, Rb;  $C^{VI}$  – S, Se) deposited on a relatively cold substrate (300 K) have an amorphous structure [1]. Amorphous layers have not an atomically smooth surface, but consist of clusters measuring from 5 to 15 nm. The contrast on the electron-microscopic images of clusters is supposed to be caused by material density changes. There are narrow and wide regions of low density between clusters for different films.

Theoretical analysis of the amorphous structure was performed in order to explain the cluster formation reasons. Two order parameters were chosen: the average angle deviation of the covalent bond from the optimal value ( $\varphi$ ) and the average interatomic distance ( $r$ ).

There are many descriptions of interatomic interactions: the Morse potential, the Van der Waals model potential, the Lenard-Jones potential. The parameter  $\varphi$  together with the use of elliptic functions gives a good description of the disorientation of highly directional covalent bonds, as well as their periodicity. The variation of the free energy with respect to the order parameters leads to a system of two Lagrange type equations. The separation of variables in these equations is a nontrivial task, so the rectangular path was chosen, consisting of three straight segments, as can be seen on Fig.1. The path runs between two

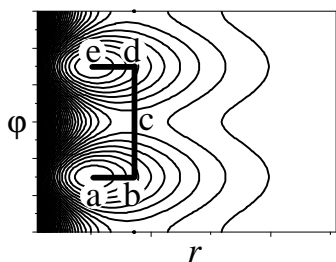


Fig. 1. The levels of potential as a function of order parameters  $r$  and  $\varphi$ ; the path of integration is also shown.

potential minima (a, e) and through saddle point (c). There are two segments (a-b and d-e) where only the interatomic distance changes and one segment (b-c-d) where only the angle varies with fixed interatomic distance. The application of this procedure of variable separation allows us to find the spatial dependence of the disordering parameters  $r$  and  $\varphi$  during the transition

from one cluster to another. Equations for the boundaries of clusters are obtained and it is shown that the boundaries of the cluster contain an increased number of disordered bonds.

1. Bilozertseva V.I., Khlyap H.M., Shkumbatyuk P.S., Dyakonenko N.L., Mamaluy A.O., Gaman D.O. Li-Be-Se semiconductor thin films: technology, structure and electrophysical properties // *Semiconductor Physics, Quantum Electronics & Optoelectronics*. – 2010. – V.13, №1. – P. 61-64.