Ring-, Branchy-, and Cage-Like As_nS_m Nanoclusters in the Structure of Amorphous Semiconductors: *ab initio* and Raman Study

R. Holomb, V. Mitsa

Research Institute for Solid State Physics and Chemistry, Uzhhorod National University, Uzhhorod 88000, Ukraine, e-mail: holomb@ukr.net, mitsa@univ.uzhgorod.ua

The conceptual statements of topological-cluster structure of non-crystalline semiconductors related with the change in the connectivity of the structure matrix and physical properties depending on the average coordination number were studied both by experimental and theoretical methods.

We here present a study of different type As_nS_m nanoclusters (n = 1-6; m = 3-6, 8, 10, 12) which realization in the amorphous structure is possible. The differences in geometry structure and chemical bonds in clusters cause the changes of their physico-chemical properties. Therefore, the formation energy, stability, electronic, optical, and vibrational properties of such clusters were calculated from the first-principles and were analyzed.

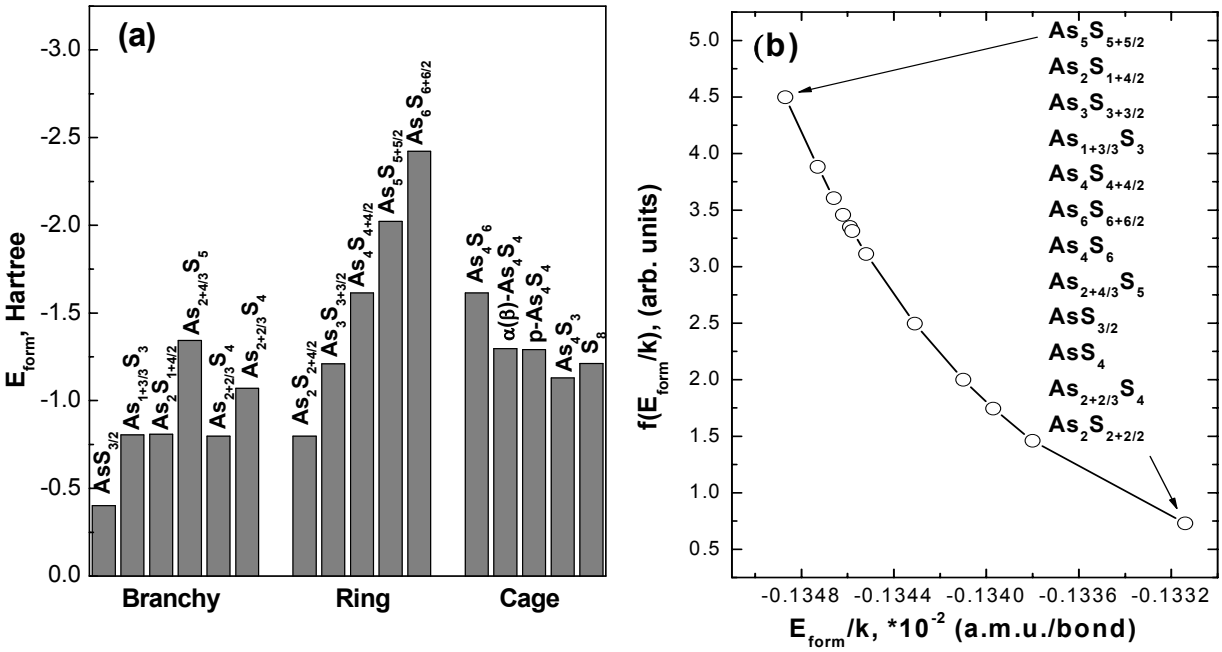

Fig. 1: Formation energy (E_{form}) and Boltzmann distribution of $E_{form.}/k$ (k is a number of bonds) values of $As_nS_m(S_8)$ clusters (b).

The physical and technological conditions under which the structure of amorphous film reaches the structure of the corresponding bulk glass or essentially differs from it have been revealed. The experimental spectra of amorphous arsenic sulphides were interpreted by using the results of *ab initio* calculations of the vibration spectra of As_nS_m nanoclusters with taking into account their relative stability.