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THE PARAMETERS LOCAL STRUCTURE OF As – Ge – Se CHALCOGENIDE GLASSES

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The chalcogenide glass-like semiconductors (ChGS) out perform other functional materials in their unique electronic properties used for applications [1 -2]. They are transparent in wide spectral region, have high photosensitivity, optical nonlinearity, high value of refraction index and also they differ from other materials by technological process simplicity at preparation of different details on their base and chemical stability[3]. Advantage of ChGS also is caused by wide region of glass formation, possibility of unlimited doping and chemical composition variation that allows us to change the structure and obtain the material with optimal parameters [1]. However, the successful realization of applied tasks requires the obtaining of material with predicted properties and optimal parameters necessary for concrete purpose. It is known, that macroscopic properties of non crystalline materials are controlled by micro-structure peculiarities, i.e. short-range order and average one in atom disposition. The change of parameters of short-range and average orders, in particular, coordination number, length and type of chemical bonds, relative part of heteropolar and homopolar bonds, correlation length and etc. can be achieved by change of chemical composition that should be reflected on structure and electron properties [4].

The investigation of local structure and physical parameters of ChGS of As – Ge – Se system is the goal of the present work. The numerical values of correlation length, quasi-period in average order region, packing coefficient, compactness, average value of atomic volume, average coordination number, limitation number, cohesion energy are obtained using X-rays diffraction method and density measurement.

The parameters of local structure (correlation length and quasi-period in average order region) are defined by carrying out of experiments by X-ray beam diffraction and density of glass-like systems As – Ge – Se. The dependence of physical parameters (density, packing coefficient, compactness, molar volume average value, lone pair electron number, cohesion energy) on average coordination number and R parameter defining the bond character between atoms is established. The compositions corresponding to chemical percolation threshold and also compositions in which the glass state is flexible, highly-stressed and isostatically stressed are established using results of Phillips-Torp and Tichy theories.

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THE OPTICAL AND ENERGY PARAMETERS OF $As_{40}Se_{60}$, $As_{40}Se_{30}Te_{30}$, $As_{40}Se_{30}S_{30}$ CHALCOGENIDE GLASSES

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The chalcogenide vitreous semiconductors (CVS) are characterized by unique physical properties, has received special attention in connection with the broad forecast for using these materials in photolithography, holography, and microelectronics [1-3]

The purpose of this paper is to study the optical properties of chalcogenide glasses, with compositions $As_{40}Se_{60}$, $As_{40}Se_{30}Te_{30}$ and $As_{40}Se_{30}S_{30}$.The optical studies provide information on the relationship of the local structure and physical properties. The transmission spectra of the thin film with compositions $As_{40}Se_{60}$, $As_{40}Se_{30}Te_{30}$ and $As_{40}Se_{30}S_{30}$ were measured in the spectral range 190-1100 nm. The optical transmission spectra exhibit interference maxima and minima in the wavelength range 600 ÷ 1100 nm. The spectral dependencies, (T(λ)) have been reestablished in the transparency area to see more clearly the interference fringes. Change of the optical and energy parameters has established by analysis of the optical transmission spectra depending on the chemical composition. It has been shown that optical constants (n_0, k, E_0, E_d, E_g) investigated materials undergo a change depending upon the chemical composition. When half of selenium atoms are replaced by sulfur atoms the numerical values of the coefficients of refractive index (n_0) and extinction (k) for $As_{40}Se_{60}$ composition are decreased, but replaced by tellurium atoms numerical values of the coefficients are increased. A numerical value of the oscillator energy (E_0), oscillator strength (E_d), the band gap (Eg), determined according Tauc methods [4] and the dispersion increases with selenium replaced by sulfur atoms, but decreases by replacing tellurium atoms. Change of the refractive index is apparently due to a change in the molar volume of matter. The participation of sulfur atoms leads to a decrease of the molar volume, but tellurium atoms leads to the growth. In the first case, the polarization ability of a substance is weakened and in the second case, it is amplified, which is reflected in the values of the refractive index. The value of cohesive energy in $As_{40}Se_{60}$ is equal 41.2 kcal/mol. This value is less than in the composition of $As_{40}Se_{30}S_{30}$ (43.15 kcal/mol), more than in the composition of $As_{40}Se_{30}Te_{30}$ (36.95 kcal/mol).Such a change in bond energies and cohesive energy leads to the observed changes in