

Structural studies of (AsSe)_{100-x} Ag_x glasses

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Abstract: Chalcogenide glasses of the As–Se system are promising materials for IR photonics due to their wide transmission window, high refractive index and photosensitivity. Silver incorporation is known to enhance nonlinear refractive index, improve physical parameters and modify short-range order in the glass network.

In present work we conducted structural studies of (AsSe)_{100-x} Ag_x compositions, where x = 0, 5, 10, 15, 20, 25. First, the composition of the glasses was verified using energy-dispersive X-ray spectroscopy (EDX) using a Quantax ESPRIT 1.8.5 on FEI NOVA NanoSEM. This was followed by X-ray diffraction (XRD) measurements performed using a Rigaku SmartLab diffractometer in parallel-beam geometry with Cu K α radiation ($\lambda = 1.5406$ Å). Raman spectroscopy measurements were carried out using a LabRAM HR spectrometer (HORIBA Scientific) in backscattering geometry at room temperature.

The obtained diffraction data for the glassy system (AsSe)_{100-x} Ag_x were used to calculate the pair distribution functions (G(r)) (Fig. 1). From the positions of the first and second maxima, the nearest-neighbour distance r_1 and the second-neighbour distance r_2 were determined. For the first coordination sphere, the interatomic distance increased with increasing silver content from 2.48 Å at x = 0 to 2.62 Å at x = 25. The corresponding values for the second coordination sphere changed from 3.69 Å at x = 0 to 3.83 Å at x = 25. The bond angle φ was calculated using the relation: $\varphi = 2 \arcsin(r_2 / 2r_1)$ and changed from 96.14° at x = 0 to 93.93° at x = 25.

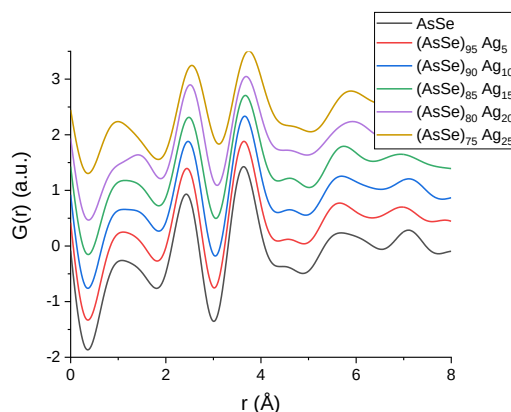


Fig. 1 Pair distribution functions (G(r)) for (AsSe)_{100-x} Ag_x compositions

An increase in silver content leads to a gradual increase of both r_1 and r_2 distances, accompanied by a decrease in the bond angle φ . This behaviour indicates structural rearrangement of the glass network and distortion of the basic AsSe₃ pyramidal units due to silver incorporation. The observed bands in the Raman spectra of the studied As–Se–Ag samples show that such glasses contain different nanophases.

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