

Structural studies of As₂S₃:AgI glasses

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Abstract: Chalcogenide glasses are widely used in photonics applications, including IR optics, sensing, optoelectronics, holography, and integrated and fiber platforms. Their optical, electrical and structural properties can be tuned by doping with different modifiers. Silver-containing chalcogenide glasses attract particular interest due to the combination of the wide glass-forming region of the As-S network and the high ionic conductivity of Ag⁺ ions. The introduction of AgI into the As₂S₃ matrix enables additional control over the structure and, consequently, the functional properties of the material.

The present work is devoted to the structural investigation of (As₂S₃)₉₅(AgI)₅ and (As₂S₃)₆₅(AgI)₃₅ glasses in comparison with pure As₂S₃. The samples were studied by X-ray diffraction. Diffraction patterns were recorded using a Rigaku SmartLab diffractometer in parallel-beam geometry with Cu K α radiation ($\lambda = 1.5406$ Å) in the 2θ range from 2° to 120° with a step of 0.05° at room temperature. The obtained diffraction curves confirm the amorphous nature of all investigated samples.

Based on the experimental XRD data, radial distribution functions (RDFs) and short-range order parameters were calculated using the RAD GTK+ software. The positions of the first (r_1) and second (r_2) maxima of the RDF were determined. The bond angle φ was calculated using the relation $\varphi = 2 \arcsin (r_2 / 2r_1)$.

Table 1. Radial distribution functions and short-range order parameters

Composition	r_1	r_2	r_2/r_1	φ
As ₂ S ₃	2.3	3.48	1.51	98.32
(As ₂ S ₃) ₉₅ (AgI) ₅	2.31	3.51	1.52	98.88
(As ₂ S ₃) ₆₅ (AgI) ₃₅	2.31	3.51	1.52	98.88

Comparison of the short-range order parameters shows that the r_1 and r_2 values for (As₂S₃)₉₅(AgI)₅ and (As₂S₃)₆₅(AgI)₃₅ are practically identical within the experimental error (± 0.01 Å). In the case of pure As₂S₃, a slight shift of r_1 is observed within the error limits. These results indicate that the introduction of AgI does not significantly disturb the short-range order of the As-S network, while structural modifications may occur at longer length scales.

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