

Section II

Chalcogenide glasses and wide – gap semiconductors

Invited Papers

Composition–structure–property relationships in amorphous sulfide thin films prepared by RF magnetron co-sputtering

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Abstract: The local atomic structure of amorphous chalcogenides decisively governs their optical properties. In this contribution, we present a systematic composition–structure–property study of amorphous sulfide thin films prepared by radio-frequency magnetron co-sputtering across the GeS_2 – Sb_2S_3 , Ga_2S_3 – Sb_2S_3 , and GeS_2 – Ga_2S_3 pseudo-binary systems, as well as the pseudo-ternary GeS_2 – Ga_2S_3 – Sb_2S_3 compositional range. RF magnetron co-sputtering enables the preparation of high-quality amorphous films over broad compositional ranges, including regions prone to crystallization in bulk form. Spectroscopic ellipsometry reveals distinct composition-dependent trends in refractive index and optical bandgap energy. In the GeS_2 – Sb_2S_3 and Ga_2S_3 – Sb_2S_3 systems, the refractive index increases systematically with increasing Sb_2S_3 content, accompanied by a corresponding decrease in E_g . In contrast, the GeS_2 – Ga_2S_3 system exhibits a nearly constant refractive index across a wide compositional range despite variations in bandgap energy. The films exhibit low absorption within the measured infrared spectral range, supporting their relevance for mid-wave and long-wave infrared applications. To clarify the microscopic origin of the observed optical trends, cluster-based density functional theory (DFT) modeling was employed to analyze Raman-active modes of representative structural motifs in Ge–S networks. The calculated spectra for corner- and edge-sharing tetrahedra, homopolar bonds, and ring- and chain-like fragments reproduce the principal experimental features and enable assignment of characteristic vibrational bands to specific local configurations.

Keywords: chalcogenides, RF magnetron co-sputtering, Mid-infrared optics