

Nanocluster-Driven Topology as a Unifying Parameter of Physical Properties in Chalcogenide Glasses

V. Mitsa^{1*}, R. Holomb^{1,2}, M. Veres¹

¹Uzhhorod National University, 89A Zankovetskoi Street, 88015 Uzhhorod, Ukraine

²Department of Applied and Nonlinear Optics, Institute for Solid State Physics and Optics, HUN-REN Wigner Research Centre for Physics, Budapest, 1121, HUNGARY

***E-mail:** v.mitsa@gmail.com

Abstract Amorphous chalcogenide glasses exhibit a wide spectrum of anomalous physical properties, including nonlinear optical response, the boson peak in the low-frequency spectra, non-Debye low-temperature thermal conductivity, complex dielectric relaxation, and pronounced photoinduced structural transformations. Despite decades of research, these phenomena are typically treated independently, and a unified microscopic interpretation remains lacking. In this report, a unified framework based on **nanocluster-driven topology** is proposed. Within this approach, chalcogenide systems such as As–S, Ge–S, and Ge–As–S are considered as structurally heterogeneous media composed of interacting nanoclusters forming medium-range order. These nanoclusters are built from fundamental structural units (AsS₃/SGe₃ pyramids and GeS₄ tetrahedra) and include “rigid”, “soft” and “defect” ring-like configurations; chain-like and branched-like with closed ends, and cage-like configurations. Their topology, connectivity, and spatial distribution define the effective structure of the glass. A key concept of the model is the presence of “**keystone nanoclusters**” [1,2] acting as topological organizing centers that determine the rigidity and stability of the network. Spectroscopic evidence supports this framework. Raman studies of glassy GeS₂ demonstrate the coexistence of nanoclusters related to both α - and β -GeS₂ crystalline phases, indicating mixed medium-range ordering. In the Raman spectra and differential spectra, characteristic bands correspond to vibrational modes of corner- and edge-sharing GeS₄ tetrahedra [3]. These results reveal that ring-like clusters dominate the structure, while defect-related units, including homopolar Ge–Ge and S–S bonds, emerge depending on preparation conditions such as quenching temperature and cooling rate. This confirms that structurally distinct nanocluster ensembles may exist even in nominally identical compositions. Experimental studies of Ge–As–S glasses further show that systems with identical mean coordination numbers exhibit significantly different nonlinear optical responses (including two-photon absorption), elastic moduli, and density depending on the compositional pathway [4]. Within the proposed framework:

- The spectroscopic and thermometric “**boson peaks**” is interpreted as a manifestation of localized and quasi-localized vibrational modes associated with nanoclusters.
- **Low-temperature thermal anomalies** arise from phonon scattering on nanocluster heterogeneities.
- **Photoinduced effects** are described as light-driven reconfiguration of nanocluster-driven topology and surface relief formation [5].

Keywords: chalcogenide glasses, elastic modulus, density, mean coordination numbers, glass structure, boson peak, low-temperature thermal anomalies, photoinduced effects.

References

1. P. Baloh et al., *J. Non-Cryst. Solids* 631 (2024) 122913
2. P. Baloh et al., *J. Non-Cryst. Solids* 600 (2023) 122040
3. V. Mitsa et al., *MIPRO Proceedings* (2014)13.
4. V. Mitsa, *Semiconductor Physics, Quantum Electronics & Optoelectronics*, 29(2026)045.
5. O. Kondrat et al., *Appl. Surf. Sci.* 518 (2020) 146240