Mass spectrometry and Raman spectroscopy of Silver-Doped $(GeS_2)_{50}(Sb_2S_3)_{50}$ of chalcogenide glasses

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Chalcogenide glasses are based mostly on sulfur, selenium, tellurium, etc. elements combined with those from the 14-15th group of the periodic system (germanium, arsenic, antimony, etc.). They are high–tech materials with strategic importance for phase change memory devices [1], optical fibers [2], fabrication of solar cells [3, 4], etc.

Analysis of chalcogenide glasses by mass spectrometry is not easy. We can't use MALDI for ionization, we have to apply laser desorption ionization or laser ablation of the materials and these are causing strong fragmentation. The possibilities of combination TOF mass spectrometry and Raman spectroscopy for the characterization of chalcogenide glasses and their structure elucidation are studied and evaluated here.

Novelty and motivation of the paper was, for example, using two very different techniques, i.e. non-destructive Raman spectrometry and destructive LDI TOF MS to follow the structure of chalcogenide glasses. In our work, the aim was to evaluate if such a combination of very different techniques might help in the characterization of silver doped chalcogenides glasses studied [5]. Also here the conclusion was that Raman is detecting basic structural units and mass spectrometry is mostly just showing their fragments. The ions observed by MS are mostly fragments of these structural units or they can be products of reactions in plasma plume (which are difficult to identify and/or eliminate).

Concluding, the mass spectrometer can be used to examine the formation of structural entities (clusters). LDI TOF MS is a powerful and useful tool to elucidate the composition of clusters formed from chalcogenide glasses determining their stoichiometry. MS is destroying the material, but the fragments represent structural entities of the studied material. Some structural units were detected by Raman spectroscopy but not observed by MS and vice versa.

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References:

[1] F. Jiang, et al., *Jpn Appl Phy*. 30, 97 (1991)
[2] J.R. Gannon. *Proc SPIE*. 266, 62-68 (1981)
[3] D.E. Carlson., et al., *Appl. Phys. Lett*. 28, 671 (1976)
[4] N. Kushwaha, et al., *J Non-Cryst Sol*. 351, 3414-3420 (2005)
[5] F. Huang, et al., *ACS Omega*. 5, 28965–28971 (2020)