Functional Materials 10, No.2 (2003)

Raman spectra of As–S(Se) glasses and sulfide (selenide) clusters

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Received October 2, 2002

The comparison results of Raman spectra of As–S(Se), As–S–Se glasses and films and of As–S(Se) type clusters are presented.

Представлены результаты сопоставления спектров комбинационного рассеяния стекол и пленок As–S(Se), As–S–Se и кластеров типа As–S(Se).

Physical properties of amorphous glasses depend on their composition and structure. Optical properties of these materials are of greatest interest due to the demand of optoelectronic industry [1]. The aim of this work is the structure research of As–S–Se system glasses basing on theoretical calculations and experimental Raman spectra.

The structure and the vibrational frequencies of some fundamental As_2S_3, $As_2S(Se)_5$, $As_4S(Se)_6$, $As_6S(Se)_9$ $As_2S_{5-x}Se_x$ type clusters were calculated applying the ab initio Hartree-Fock method with LANL2DZ base set.

The preparation method of $As_{40}S_{60-x}Se_x$ glasses (x = 0, 20, 40, 60) is described in [2]. Raman spectra of the samples were measured using a Fourier Transformation (FT) Raman spectrometer (IFS/FRA 106, Bruker). The Raman spectra were excited using a laser beam λ = 1064 nm of 50 mW output power. The Raman spectrometer resolution was 1 cm^{-1}.

The frequency spectra of As_2S_5 and As_2Se_5 clusters under the sequential substitution of sulfur by selenium were compared to the FT Raman spectra of the As–S–Se system. The model calculations show that an $As_2S(Se)_5$ chain cluster with triangles at the chain ends (Fig. 1) is more favorable. For sulfur bridge atoms in $As_2S_{5-x}Se_x$ cluster, 307, 311, 350, 369 cm^{-1} bands are the most characteristic (Table). For selenium bridge atom, such bands are 200, 214, 221, 248, 257 cm^{-1} ones (Table).

It is seen from the Raman spectra of $As_{40}S_{60-x}Se_x$ glasses (Fig. 2) that as the selenium content rises, the 250 cm^{-1} band intensity increases and the band shifts towards lower frequencies. The intensity of 340 cm^{-1} band decreases and its maximum shifts to higher frequencies. These facts are

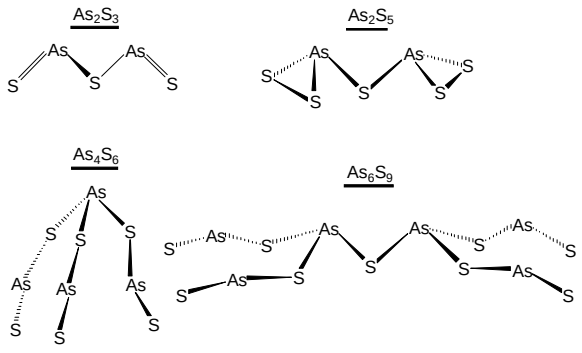

Fig. 1.