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The boson peak and the first sharp diffraction peak in $(As_2S_3)_x(GeS_2)_{1-x}$ glasses

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Abstract. The parameters of the boson peak (BP) and the first sharp diffraction peak (FSDP) in $(As_2S_3)_x(GeS_2)_{1-x}$ glasses measured using high-resolution Raman spectroscopy and high-energy synchrotron X-ray diffraction measurements are examined as a function of x. It has been found that there is no correlation between the positions of BP and FSDP. The BP position shows a nonlinear composition behavior with a maximum at about $x = 0.4$, whereas the FSDP position changes virtually linearly with x. The intensities of both BP and FSDP show nonlinear composition dependences with the slope changes at $x = 0.4$, although there is no direct proportionality. Analysis of the partial structure factors for the glasses with $x = 0.2$, 0.4 and 0.6 obtained in another study has shown that the cation-cation atomic pairs of Ge–Ge, Ge–As and As–As make the largest contribution to FSDP, where the Ge–Ge and Ge–As pairs are dominant.

Keywords: chalcogenide glasses, Raman spectroscopy, X-ray diffraction, boson peak, first sharp diffraction peak, molecular structural units.

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1. Introduction

There have been a few studies aimed to answer the question about a possible correlation between the boson peak (BP) or low-frequency vibrations in the Raman spectrum and the first sharp diffraction peak (FSDP) in the structure factor $S(Q)$ for network glasses. It has been concluded in Refs. [1–6] that BP and FSDP originate from the medium-range structural correlations. Novikov and Sokolov [1, 2] suggested that there is a "universal" correlation between the positions of the BP and FSDP in glasses. On the other hand, Börjesson *et al.* [7] showed the opposite trends for the positions of BP and FSDP. Ribeiro [8] showed that in supercooled ionic liquids the correlation length related to the BP does not change with the length of the alkyl chain in imidazolium cations, in contrast to the position of the FSDP observed in neutron and X-ray scattering measurements. Uchino [9] suggested that in amorphous silica, the frequency in the BP maximum is compared with the crossover between weak- and strong-scattering regimes, often called as the Ioffe–Regel crossover, but the relation between the acoustic modes and boson peaks remains to be clarified. Baldi *et al.* [10] resolved this problem showing that for vitreous silica the Ioffe–Regel frequency is very close to the BP frequency. According to the Uchino [9], the first sharp diffraction peak covers only a small part of the medium range order scale, while localized vibrational properties including boson peak are extended over the whole medium range order scale up to a limit of the Ioffe–Regel crossover. On the other hand, Nakamura *et al.* [11] reported on the basis of inelastic neutron scattering measurements by using vitreous silica that the Ioffe–Regel condition is applicable to the FSDP position. Interconnection of hysteresis of low temperature thermal conductivity, Boson peak in glassy As_2S_3 and low frequency As_nS_m nanocluster vibrations was considered in [12]. FSDP has anomalous dependences on temperature, pressure and composition [13]. Different controversial interpretations of FSDP imply necessity of further studying its nature. The better understanding of correlations between their structural and macroscopic properties and information on the short-range order structure of chalcogenide glasses is needed. This was the main motivation to study As_2S_3–GeS_2 line of chalcogenide glasses. The composites based on these chalcogenide glasses can be used for direct recording the optical elements [14–16].

Chalcogenide glasses along the As_2S_3–GeS_2 line are good candidates to study a relationship of BP and FSDP due to a mixture of two kinds of molecular structural units – $AsS_{3/2}$ pyramids and $GeS_{4/2}$ tetrahedra. In this work, the parameters of BP and FSDP obtained using high-resolution Raman spectroscopy and high-energy synchrotron XRD measurements, respectively, are investigated for $(As_2S_3)_x(GeS_2)_{1-x}$ glasses with x = 0.0, 0.1, 0.2, 0.4, 0.6, 0.8, 1.0.

2. Experimental details

$(As_2S_3)_x(GeS_2)_{1-x}$ bulk glasses were prepared using the standard melt-quenching route [17]. After synthesis, the ingots were cut into the disks of about 1 mm thickness, which then were polished to a high optical quality. Before experimental measurements, the samples were annealed at 20…30 K below glass transition temperature T_g to remove possible mechanical stresses formed after synthesis.

The Raman spectra were excited with the 647.1 nm Kr^+ laser line at the power density close to 40 mW by using pseudo-backscattering geometry. The scattered light was detected using a cooled photomultiplier and analyzed by a SPEX 1403 double monochromator operating at the spectral bandpass close to 1.5 cm^{-1}. The Raman spectra were recorded separately in two configurations, corresponding to parallel (VV – vertical-vertical) and crossed (VH – vertical-horizontal) polarizations between incident and scattered light.

The high-energy synchrotron XRD experiments were performed at the synchrotron experimental station BW5 at HASYLAB, DESY (Hamburg, Germany). The measurements were carried out in transmission geometry with the photon energy 98.9 keV. Raw data were corrected for the detector dead-time, polarization, absorption and variation of the solid angle in detector [18]. The scattering intensity was converted into the coherent scattering intensity per atom in electronic units by using the generalized Krogh–Moe–Norman method [19, 20]. The Compton scattering was corrected using the values given by Balyuzi [21]. Faber–Ziman [22] total structure factor $S(Q)$ was finally calculated.

3. Results

The polarized-VV and depolarized-VH Raman spectra of $(As_2S_3)_{0.2}(GeS_2)_{0.8}$ glass are shown in Fig. 1 as an example. From the comparison of the VV and VH spectra, the following features in respect to the boson peak can be noted: (i) the low-frequency vibrational range of the Raman spectrum in both VV and VH configurations is characterized by the presence of the excess quasi-elastic light scattering well fitted using Theodorakopoulos–Jackle (T–J) model [23] as shown schematically by lines with arrows in the insert to Fig. 1; and (ii) larger excess quasi-elastic light scattering is found for the VV configuration than for the VH one, and, thus, for correct analysis of the boson peak or low-frequency vibrational excitations, the Raman spectra recorded in the VH configuration should be taken into account.

Fig. 2 shows the depolarized-VH Raman spectra for the investigated $(As_2S_3)_x(GeS_2)_{1-x}$ normalized to the intensity of the main molecular band at 342 cm^{-1} and the ratio of the BP to the main molecular peak at this frequency (I_{bos}/I_{mol}) as a function of composition x. The authors [4–6] suggested that the ratio I_{bos}/I_{mol} is attributed to the degree of disorder on the medium range scale. One can see from Fig. 2 that the dependence of $I_{bos}/I_{mol} = f(x)$ displays nonlinear composition behavior with a pronounced minimum near the composition with $x = 0.4$. It should be noted that this nonlinear dependence of the I_{bos}/I_{mol} ratio has not been observed for $(As_2S_3)_x(GeS_2)_{1-x}$ glasses in works [5, 6], probably due to a limit number of the alloys studied.

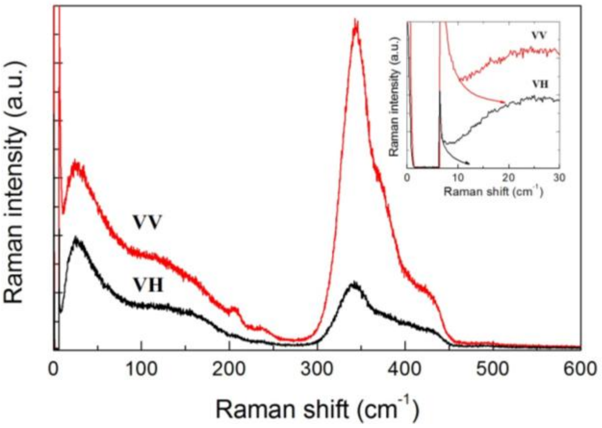

Fig. 1. The polarized-VV and depolarized-VH Raman spectra of $(As_2S_3)_{0.2}(GeS_2)_{0.8}$ glass, taken as an example, with the excess quasi-elastic light scattering in the low-frequency vibrational region well fitted using T–J model [26] as shown schematically by lines with arrows in the insert (see the text for details).

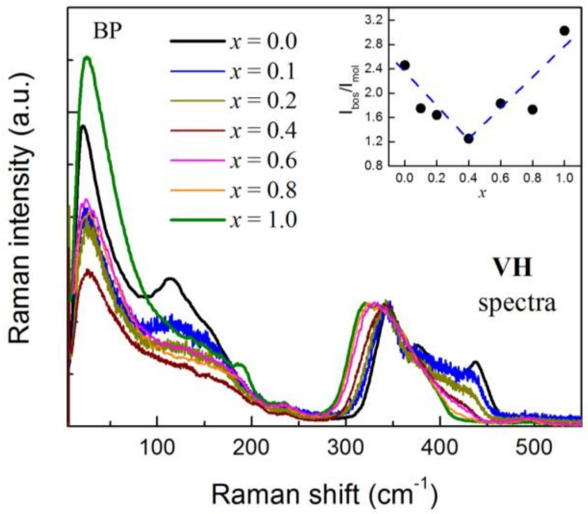

Fig. 2. The depolarized-VH Raman spectra for the investigated glasses in the $(As_2S_3)_x(GeS_2)_{1-x}$ system (x = 0.0, 0.1, 0.2, 0.4, 0.6, 0.8, 1.0) normalized to the intensity of the main molecular band. The insert shows the ratio of the boson peak (BP) to the main molecular peak (I_{bos}/I_{mol}) as a function of composition x. The dashed lines are drawn as a guide for the eye.

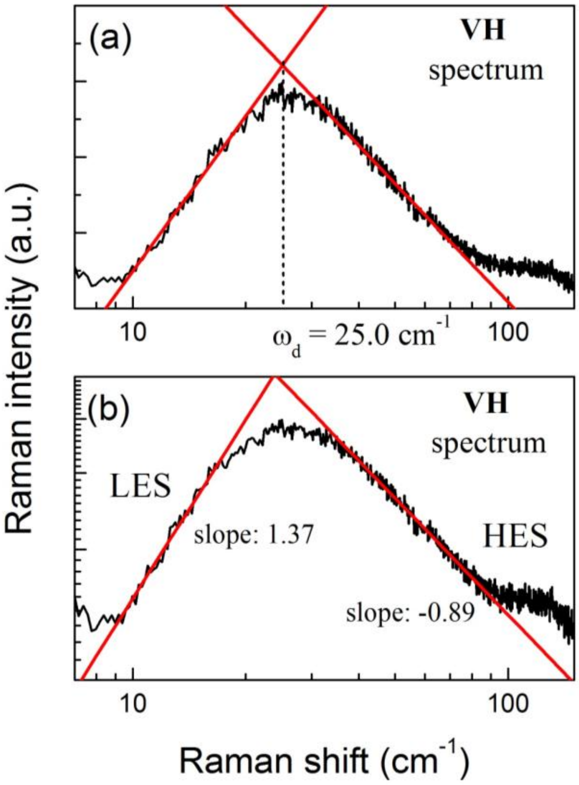

Fig. 3. (a) Linear-log and (b) log-log depolarized-VH Raman spectra showing determination of the crossover frequency ω_d and low and high-energy slopes (LES and HES) of the boson peak (BP) taken for the $(As_2S_3)_{0.2}(GeS_2)_{0.8}$ glass as an example. The crossover frequency ω_d can be considered [39] as the most corresponding one to the BP frequency ω_{bos} (*i.e.*, $\omega_d \equiv \omega_{bos}$).

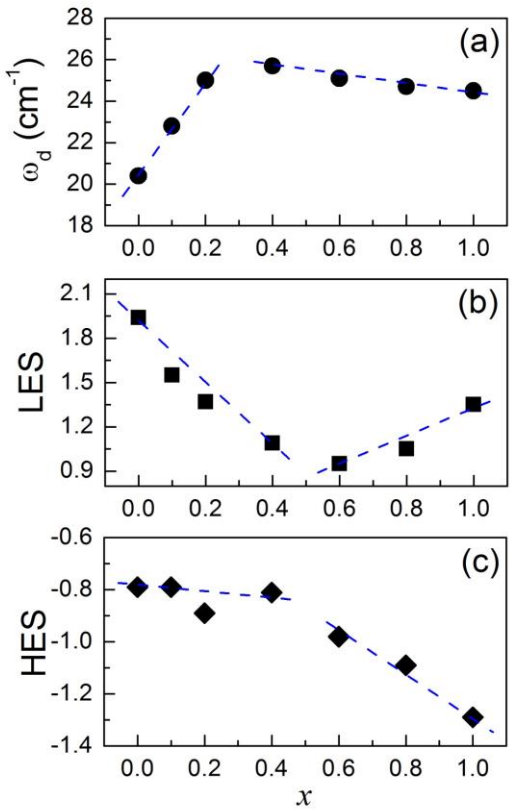

Fig. 4. (a) Crossover frequency ω_d ($\equiv \omega_{bos}$), and (b) low-energy slope (LES) and (c) high-energy slope (HES) of the boson peak (BP) for the investigated glasses in the $(As_2S_3)_x(GeS_2)_{1-x}$ system as a function of composition x. The dashed lines are drawn as a guide for the eye.

Following to the works [4, 6], one can estimate the crossover frequency ω_d, which is considered as the most corresponding frequency to the boson peak ω_{bos} (*i.e.* $\omega_d \equiv \omega_{bos}$), in the $I(\omega) - \log_{10}\omega$ scale as well as the low and high-energy slopes (LES and HES) of the boson peak in the $\log_{10}I(\omega) - \log_{10}\omega$ scale. The linear-log and log-log plots for the depolarized-VH Raman spectra of $(As_2S_3)_{0.2}(GeS_2)_{0.8}$ glass and determination of the ω_d and LES and HES values are shown as an example in Fig. 3. The composition dependences of these parameters for $(As_2S_3)_x(GeS_2)_{1-x}$ glasses are plotted in Fig. 4. One can see that ω_d, LES and HES change practically linearly, but with different slopes, in two composition intervals approximately separated by $x = 0.4$, thus being in a good agreement with the behavior of $I_{bos}/I_{mol} = f(x)$ in Fig. 2.

The first sharp diffraction peak exists in the low Q part of the structure factor $S(Q)$ for all glasses studied in this work, and its intensity as well as position exhibit a strong composition dependence as shown in Fig. 5. The ratio of the FSDP height to the value at the first minimum right to FSDP $S(Q)_{\max}/S(Q)_{\min}$ increases from ~1.9 to ~4.3 and its position shifts from 1.26 Å^{-1} to 1.03 Å^{-1} with increasing GeS_2 content in $(As_2S_3)_x(GeS_2)_{1-x}$ glasses. The FSDP position varies nearly linearly with x, whereas

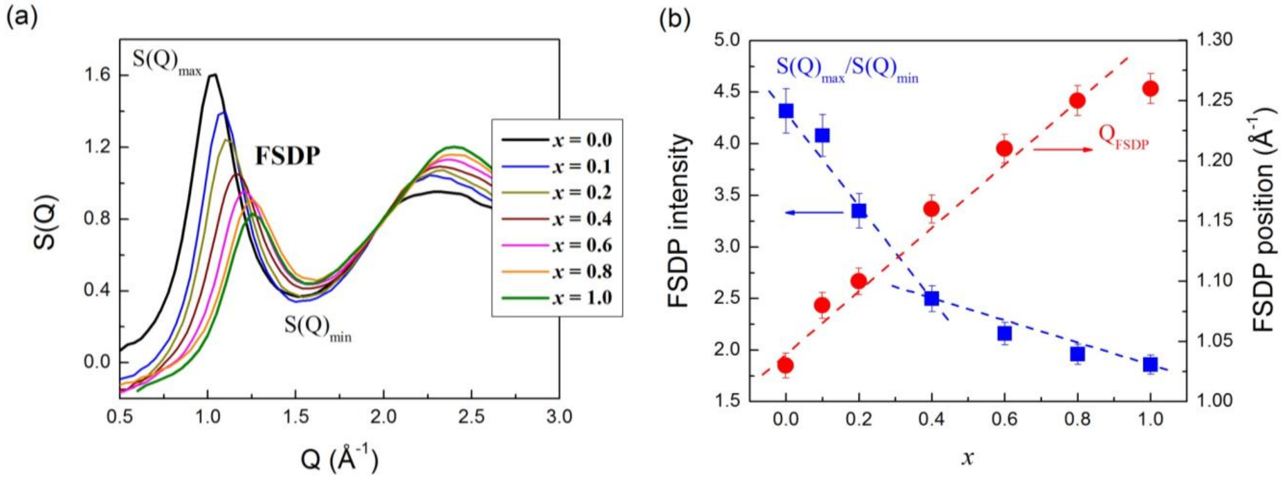

Fig. 5. (a) Low-Q part region of the total structure factors $S(Q)$ for the investigated glasses in the $(As_2S_3)_x(GeS_2)_{1-x}$ system (x = 0.0, 0.1, 0.2, 0.4, 0.6, 0.8, 1.0) (the first sharp diffraction peak is marked by FSDP) and (b) the intensity (squares) and position (cycles) of the FSDP as a function of composition x (the FSDP intensity is taken as the ratio of intensities in the peak maximum to the tail of the peak ($S(Q)_{max}/S(Q)_{min}$)). The dashed lines are drawn as a guide for the eye.

the FSDP intensity shows a nonlinear trend with different slopes within the composition range $0.0 \le x < 0.4$ (GeS_2-rich glasses) and $0.4 < x \le 1.0$ (As_2S_3-rich glasses). Similarly, a linear composition dependence of the FSDP position and nonlinear dependence of the FSDP intensity have been observed for $Ge_xAs_xS_{100-2x}$ glasses with $15 \le x \le 33.3$ [24] and $Ge_xAs_yS_{100-x-y}$ glasses with $35 \le x + y \le 65$ [25].

In order to identify the contribution of each atomic pairs to the FSDP occurrence in a multicomponent glass the corresponding partial structure factors should be resolved. It has been recently made for the $(As_2S_3)_x(GeS_2)_{1-x}$ glasses in the devoted study by using the reverse Monte–Carlo (RMC) simulation technique [29]. The partial structure factors $S_{ij}(Q)$ for $(As_2S_3)_x(GeS_2)_{1-x}$ glasses with x = 0.2, 0.4 and 0.6 are shown in Fig. 6. It can be seen that the main contribution to FSDP is due to the cation-cation atomic pairs Ge–Ge, Ge–As and As–As, where the Ge–Ge and Ge–As pairs seem to be dominant.

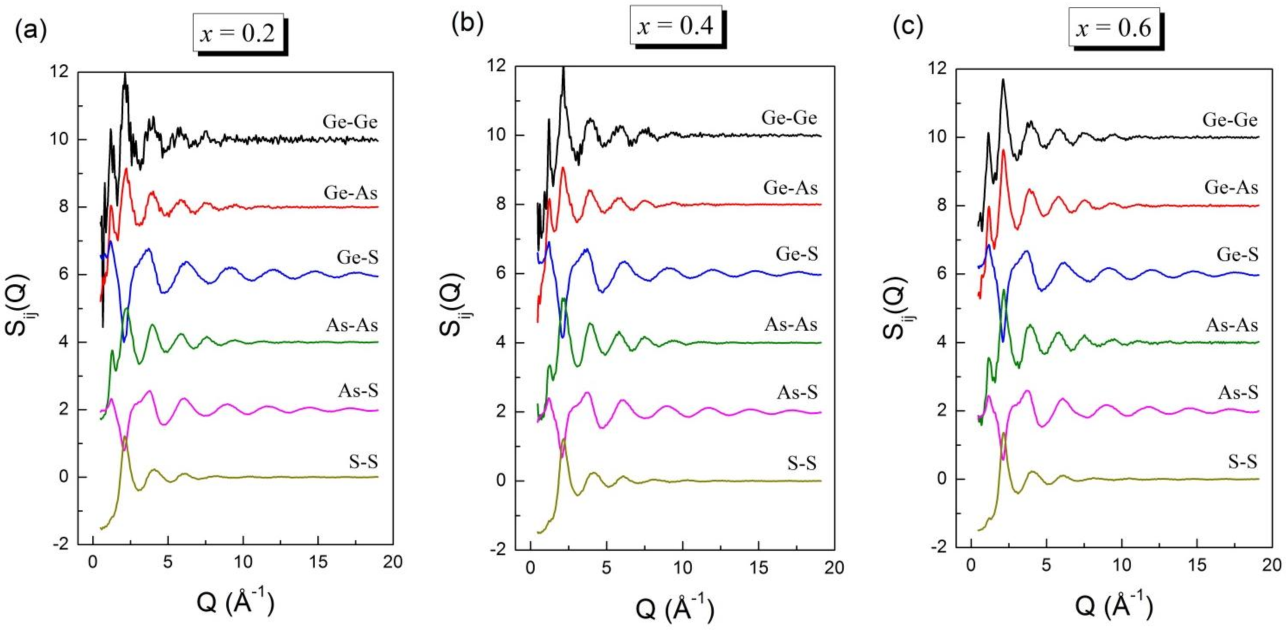

Fig. 6. Partial structure factors $S_{ij}(Q)$ for the selected glasses in the $(As_2S_3)_x(GeS_2)_{1-x}$ system with x = 0.2 (a), 0.4 (b), and 0.6 (c). The curves are shifted for clarity.

4. Discussion

To our knowledge, a possible relationship between low-frequency (boson) peak in Raman spectra and FSDP in network glasses has firstly been reported by Novikov and Sokolov [1, 2]. It has been found out that changes of the position as well as intensity of BP and FSDP show good correlation. On the other hand, Börjesson *et al.* [7] observed opposite trends of the positions of BP and FSDP of oxide glasses, structurally modified on the medium (intermediate) range order scale, and suggested that the relationship reported by Novikov and Sokolov [1, 2] seems to be too simple.

As it can be seen from Figs 4a and 5b, the position of BP $\omega_d (\equiv \omega_{bos})$ shows a nonlinear composition dependence in $(As_2S_3)_x(GeS_2)_{1-x}$ glasses, while the position of FSDP changes practically linearly with x. This supports the conclusion of Börjesson *et al.* [7] suggesting a failing correlation of the BP and FSDP positions. It is interesting that there is correlation between the composition dependences of the intensities of BP and FSDP, although not a proportionality. Indeed, both parameters show a change of slope (maximum and kink, respectively) in the vicinity of the alloy with $x = 0.4$. This calls for additional studies upon consideration of the Ioffe–Regel condition for the chalcogenide glasses and recent theoretical approaches.

The RMC-based finding that the cation-cation atomic pairs make the largest contribution to FSDP agrees with the Elliott's void-based model for FSDP [26, 27], in which FSDP is a chemical-order pre-peak due to interstitial volume around cation-centered structural units, and with Bychkov's *et al.* [28] explanation for FSDP on the basis of the network-forming cation-cation (NFC) correlations.

5. Conclusions

The parameters of the BP and the FSDP parameters in $(As_2S_3)_x(GeS_2)_{1-x}$ glasses have been studied as a function of composition x. The BP position shows nonlinear composition behavior over the whole composition range with an extremum or a kink in the vicinity of the alloy with $x = 0.4$ as well as low- and high-energy slopes of the BP. On the other hand, a linear composition dependence is observed for the FSDP position. The BP and FSDP intensities show a change of the slope and extremum at $x = 0.4$. This suggests that a further study of the relationship between BP and FSDP and its nature is needed. Comparison of the partial structure factors for the glasses with $x = 0.2$, 0.4 and 0.6 obtained by RMC modeling elsewhere shows that the cation-cation atomic pairs make the largest contribution to FSDP. This is in agreement with void-based model for FSDP after Elliott [26, 27] and NFC-correlations suggested by Bychkov *et al.* [28].

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Бозонний пік та перший різкий дифракційний пік у стеклах $(As_2S_3)_x(GeS_2)_{1-x}$

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Параметри бозонного піка та першого різкого дифракційного піка в стеклах $(As_2S_3)_x(GeS_2)_{1-x}$, виміряні за допомогою КР-спектроскопії з високою роздільною здатністю та рентгенівської дифракції високих енергій синхротрона, досліджено як функцію x. Установлено, що між позиціями бозонного піка та першого різкого дифракційного піка немає взаємозв'язку. Положення бозонного піка показує нелінійну поведінку композиції з максимумом приблизно при $x = 0,4$, тоді як положення першого різкого дифракційного піка змінюється практично лінійно з x. Інтенсивності піків показують нелінійні залежності складу із змінами нахилу при $x = 0,4$, хоча прямої пропорційності немає. Аналіз структурних факторів для зразків $x = 0,2$, 0,4 та 0,6, отриманий в іншому дослідженні, показує, що катіон-катіонні атомні пари Ge-Ge, Ge-As та As-As роблять найбільший внесок у перший різкий дифракційний пік, де домінують пари Ge-Ge та Ge-As.

Ключові слова: халькогенідні стекла, КР-спектроскопія, рентгенівська дифракція, бозонний пік, перший різкий дифракційний пік, молекулярні структурні одиниці.