

Local atomic structure of Ge-Se-Te-(Ho) glasses

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Chalcogenide glasses belong to the group of glassy semiconductors having p-type electrical conductivity, are characterized by the value of the forbidden band $E_g \approx 2$ eV and are transparent in the middle and far IR region of spectra. They are promising materials for telecommunication applications, integrated optics, biomedicine and thermal imaging because they are transparent over a wide range of wavelengths in the infrared region, they possess high refraction index and low phonon energies. Optical and electrical properties of $\text{Ge}_{20}\text{Se}_{80-x}\text{Te}_x$ glass systems for $x \in (0, 15)$ were presented in previous studies [1, 2]. In this work we focused on local atomic structure of $\text{Ge}_{20}\text{Se}_{75}\text{Te}_5$ glasses doped with 1500 ppm and 2000 ppm of Ho.

X-ray diffraction (XRD) experiments using high-energy photons were performed at the P02.1 undulator beamline of the PETRA III positron storage ring at DESY/HASYLAB (Hamburg, Germany). The diffraction patterns were acquired in transmission mode. The energy of the synchrotron radiation was set to 59.8 keV, which corresponds to the wavelength of $\lambda=0.2076$ Å. The samples were illuminated by an incident beam having a cross section of 0.5×0.5 mm². Two-dimensional XRD patterns were collected using a fast image plate detector Perkin Elmer 1621 (2048 \times 2048 pixels, 200×200 μm^2 pixel size, intensity resolution of 16 bit) carefully mounted orthogonal to the X-ray beam. The sample-to-detector distance was set to 324 mm which corresponds to q -range ($q = 4\pi \sin(\theta)/\lambda$ where 2θ is the scattering angle) up to 20 Å⁻¹. CeO_2 standard was used to calibrate the sample-to-detector distance and tilt of the imaging plate relative to the beam path. Two-dimensional XRD patterns were integrated to the q -space using the software package FIT2D [3]. The data were then converted to the total structural function, $S(q)$, using standard procedures described in [4]. The integrated data were corrected for sample absorption, fluorescence contribution, inelastic scattering using PDFgetX2 software [5].

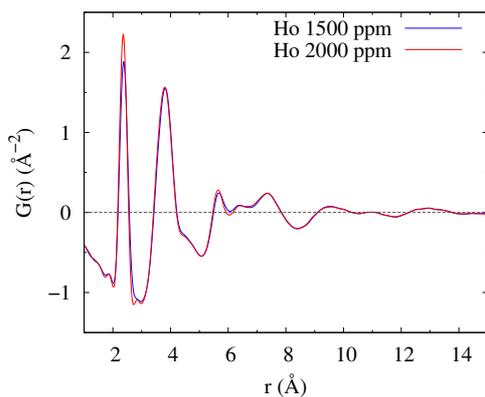


Figure 1: Comparison of reduced pair distribution functions $G(r)$ for $\text{Ge}_{20}\text{Se}_{75}\text{Te}_5$ glasses doped with Ho.

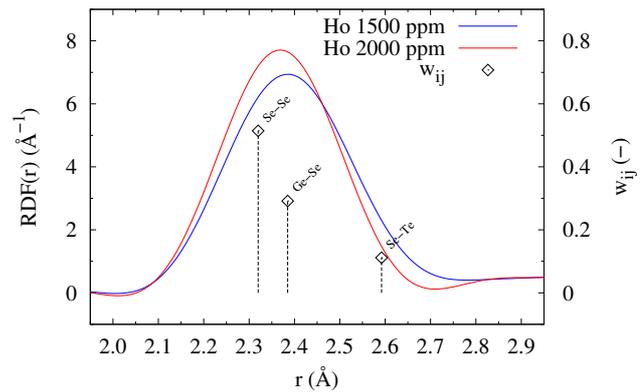


Figure 2: Comparison of the first coordination shell on radial distribution functions $RDF(r)$ for $\text{Ge}_{20}\text{Se}_{75}\text{Te}_5$ samples doped with Ho.

Figure 1 shows reduced pair distribution functions, $G(r)$, for $\text{Ge}_{20}\text{Se}_{75}\text{Te}_5$ glasses doped with Ho (1500 and 2000 ppm). Pair distribution functions $G(r)$ exhibit rather broad and rapidly decaying oscillations which are fingerprint of missing long-range order. Figure 2 shows detailed view of radial distribution functions, $RDF(r)$, depicting the first coordination shell (the nearest atomic

neighbourhood) for different level of doping. As can be seen from Fig.2, changing level of doping affects the nearest atomic neighbourhood of Ge-Se-Te-(Ho) glasses. In Ge-Se-Te glass there are six atomic partials, i.e. Se-Se, Se-Ge, Se-Te, Ge-Ge, Ge-Te and Te-Te. Depending on concentration and X-ray scattering power of Ge, Se and Te, atomic pairs contribute with different weights w_{ij} to the total $S(q) = \sum w_{ij}(q)S_{ij}(q)$. It should be noted here that due to substantially lower content of Ho, atomic pairs with Ho are having very small X-ray scattering weights. Atomic partials Se-Se, Se-Ge and Se-Te are most dominant one and determine the shape of the first coordination shell (see Fig.2). In order to get quantitative comparison profile of the first coordination shell was decomposed using three Gaussians. From obtained results one can see that higher level of Ho doping implies shortening of the interatomic distances. Also corresponding distributions of bond lengths become narrower when increasing level of Ho doping. Furthermore one can see that higher level of Ho doping implies slightly higher mean atomic density and coordination number which suggest better atomic packing.

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