Structural correlations of Ge20Se80−xTex glasses based on reverse Monte Carlo simulation

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Abstract:

Bulk chalcogenide Ge20Se80−xTex (where x = 0, 10, 20 and 30 at.%) glasses were prepared using the meltquench technique. The total structure factors of these alloys are obtained from the X-ray scattering data in the momentum transfer interval 0.61 ≤ K ≤ 16.45 Å⁻¹. From reverse Monte Carlo (RMC) simulations of the X-ray scattering data, the short and intermediate-range order parameters are obtained. The simulations are useful to compute the partial pair distribution functions, g_{ij}(r), and the partial structure factors, S_{ij}(K). In Te-rich glass, the first sharp diffraction peak (FSDP) appears as a shoulder, instead of a peak for others, confirms that Se–Se bonds in addition to Ge–Ge bonds are responsible for the intermediate-range order inside these glasses. The partial coordination numbers and the bond angle distributions within the first coordination shell have been calculated. The ratio of the first to second peak positions (r₁/r₂) and the corresponding bond angle (θ) have confirmed that the Ge(Se₁/2)₄ tetrahedra, connected by Se–Se chains, can be considered as the main building units inside the investigated glasses.

Keywords:

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