Structure of Ge-Se glasses

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Abstract

Chalcogenide glasses (those containing S, Se or Te) can be formed over a wide compositional range, and feature networks that are built from a rich variety of structural motifs that include homopolar bonds and edge sharing tetrahedral units. It is therefore a formidable challenge to solve the structure of these materials by diffraction methods, especially when the chemical species in a given material have similar neutron scattering lengths or x-ray form factors. In this talk, I will present new results on the structure of Ge-Se based glasses as obtained by using the method of neutron diffraction with isotope substitution. I will show how the technique can be used to gain site-specific information on the coordination environments of the chemical species over multiple length scales, thus providing essential information on the glass structure. I will show how advances in neutron diffraction now make it possible to measure the full set of partial structure factors for an enhanced range of glassy materials. The results are compared to those obtained from first-principles molecular dynamics simulations. Future challenges for experiment and simulation are discussed.

Keywords: Chalcogenide glasses, Neutron diffraction, partial structure factors, glass structure

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