Short range order in covalent glasses – problems and possible solutions

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Chemical short range order and accurate values of coordination numbers in amorphous alloys can only be obtained if the partial pair correlation functions are reliably separated. Among the factors determining the 'strength' (informativeness) of experimental data the most fundamental and most neglected is sampling theorem [1] that defines the real real space resolution. Sampling theorem is used to show that it is impossible to separate the partial pair correlation functions of binary telluride glasses using neutron and X-ray diffraction only. However, in several cases EXAFS offers a straightforward way to solve this problem. Coordination constraints can also be used to decrease the uncertainty of structural parameters. The reliability of various RMC models of binary Ge-Te, As-Te, Ge-Se and As-Se glasses is discussed and glassy germanium tellurides (from binary Ge-Te to Ge-Ag-I-Te) are used to demonstrate how RMC can combine diffraction, EXAFS and coordination constraints.

Reference

[1] C. E. Shannon, Proc. of the Institute of Radio Engineers. 37, 10 (1949); reprint edition: Proc. IEEE 86, 447 (1998) DOI: 10.1109/JPROC.1998.659497