

New geometrical modelling of B₂O₃ and SiO₂ glass structures

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New geometrical modelling of glass structure employing 'local oxygen packing number (LOPN)' has been developed. This modelling enables the quantification of the variation in local structure in terms of oxygen packing. This new method was applied to analyse the structures of SiO₂, B₂O₃ and boric acid systems. The analysis of LOPN for the SiO₂ system shows that each structure can be classified into one of three different packing groups. Moreover, in terms of LOPN, the densification of silica glass is found to increase the fraction of coesite-like denser fragments taking the place of quartz-like and cristobalite-like fragments, although the packing group remains the same. B₂O₃ and boric acid systems can also be explained in terms of these three different packing groups. However, in contrast to the SiO₂ system, most of these borate structures have characteristics of two different groups. The differences in LOPN can be related to the difference in dimensionality of packing, as exhibited by: (1) coordination numbers of cations and anions, and (2) the existence of super-structural units such as the boroxol ring, or low dimensional structures such as chain packing. It is also revealed that the local oxygen packing can differ from place to place even in one structure, and the LOPN is a more powerful tool to investigate structures than the conventional concept of overall packing density.
