XAFS Studies of Alkaline-Earth Borate Glasses

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Abstract

The local structure obtained from calcium K-edge XAFS experiments in CaO-B₂O₃ glasses is described. The average coordination number of oxygen around Ca²⁺ ions and the mean distance for Ca-O are found to be approximately 6 and 2.40~2.41Å. The Ca²⁺ ions have a disordered octahedral geometry and a strong preference to residence in vicinity of negatively charged non-bridging and bridging oxygen in the large cages of the B-O network structure. The XAFS results are in good agreement with MD simulation results.

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