

Abstract Submitted  
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**Structural transitions in vitreous B2O3 under pressure** LIPING HUANG, JOHN KIEFFER, Department of Materials Science and Engineering, University of Michigan — We have studied the nature of structural transitions in B2O3 glass under pressure using molecular dynamics (MD) simulations, based on a coordination-dependent charge transfer potential. This potential model allows the charges on atoms to re-distribute upon the formation and rupture of chemical bonds, and accommodates multiple coordination states during the course of simulations. Our MD simulations show that the boroxol rings in vitreous B2O3 break up when subject to pressure, which explains the disappearance of the breathing mode in the experimental Raman spectrum of B2O3 glass under pressure. Excellent agreement is found between simulations and Brillouin scattering results in terms of the sequence of polyamorphic transitions during compression-decompression cycle and the amount of permanent densification in vitreous B2O3 after pressure release. The polyamorphic transitions in three-coordinated B2O3 glass involve transitory four-coordinated boron atoms at high pressures, while coordination change is not necessary for compaction of four-coordinated silica glass.

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