

Abstract Submitted  
for the MAR05 Meeting of  
The American Physical Society

**Structural transitions in vitreous B<sub>2</sub>O<sub>3</sub> under pressure** LIPING HUANG, JOHN KIEFFER, Department of Materials Science and Engineering, University of Michigan — We have studied the nature of structural transitions in B<sub>2</sub>O<sub>3</sub> 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 B<sub>2</sub>O<sub>3</sub> break up when subject to pressure, which explains the disappearance of the breathing mode in the experimental Raman spectrum of B<sub>2</sub>O<sub>3</sub> 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 B<sub>2</sub>O<sub>3</sub> after pressure release. The polyamorphic transitions in three-coordinated B<sub>2</sub>O<sub>3</sub> 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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Date submitted: 01 Dec 2004

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