

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Visualization of fracture precursors in vitreous silica: study of under- and over coordinated ions FRANK JONES, ROMULO OCHOA, DEBORAH KNOX, The College of New Jersey — We have conducted classical molecular dynamics fracture studies of vitreous silica. A new visualization program was designed to observe the fracture process of the sample as a whole. The program also allows users to highlight and focus on the under- and over coordinated oxygen and silicon ions. A BKS potential was utilized to model the ionic interactions. DL-POLY* was the program used to perform simulations. Amorphous silica samples were generated at high temperatures; through a series of quenching and equilibration periods vitreous silica was obtained at room temperature. This method resulted in samples having, initially, a number of under- and over coordinated ions (less than one percent of all ions) that were randomly distributed. Radial distributions functions were obtained to verify the amorphous structure of the samples. Stress was applied by uniaxially straining the samples at various rates. As a sample was strained there was an increase in under coordinated ions with seemingly no correlation to the region where the sample would break. In all our simulations the under coordinated ions concentrated in the vicinity of the breakage region a few picoseconds before fracture occurred. *CCLRC Daresbury Laboratory, UK

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Date submitted: 23 Nov 2008

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