

Abstract Submitted  
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**Multiscale Modeling of Fracture in an SiO<sub>2</sub> Nanorod**<sup>1</sup> ADITI MALLIK, KEITH RUNGE, KRISHNA MURALIDHARAN, JAMES DUFTY, University of Florida — The fracture of a 108 particle SiO<sub>2</sub> nanorod under uniaxial strain is described using an NDDO quantum mechanics. The stress – strain curve to failure is calculated as a function of strain rate to show a domain that is independent of strain rate. A pair potential for use in classical MD is constructed such that the elastic portion of the quantum curve is reproduced. However, it is shown that the classical analysis does not describe accurately the large strain behavior and failure. Finally, a composite rod is constructed with a small subsystem described by quantum mechanics and the remainder described by classical MD <sup>1</sup>. The stress – strain curves for the classical, quantum, and composite rods are compared and contrasted. 1. “Multiscale Modeling of Materials – Concepts and Illustration”, A. Mallik, K. Runge, J. Dufty, and H-P Cheng, cond-mat 0507558.

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