

Abstract Submitted  
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**First-principles study of the amorphization of stishovite by isotropic volume expansion** MASA AKI MISAWA, FUYUKI SHIMOJO, Kumamoto University, RAJIV K. KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Simple synthesis of ceramics with high hardness and high toughness from Earth-abundant materials is one of the most important issues in materials science. Nishiyama et al. synthesized nano-crystalline stishovite with extremely high toughness and high hardness via compression and decompression of silica, and proposed fracture-induced amorphization mechanisms for the toughening [1]. Furthermore, it was shown that the toughening mechanisms are effective even in nanoscale order [2]. Our first-principles molecular dynamics simulations have shown rapid amorphization of stishovite within picoseconds under increasing volume, thus substantiating the proposed amorphization mechanisms. Furthermore, we have calculated the critical stress, energy difference, and energy barrier for the crystalline-to-amorphous structural transition. [1] N. Nishiyama et al., Scientific Reports 4, 6558 (2014). [2] K. Yoshida et al., Scientific Reports 5, 10993 (2015).

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