

Atomistic Modeling of Mechanical Loss in Amorphous Oxides.

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Abstract:

The mechanical and optical loss in amorphous solids, described by the internal friction and light scattering susceptibility are investigated using classical, atomistic molecular dynamics simulation. We implemented the trajectory bisection method and the non-local ridge method in DL-POLY molecular dynamics simulation software. These methods were used to locate the different local potential energy minima that a system visits through an MD trajectory and the transition state between any two consecutive minima. From the distributions of the barrier height and asymmetry, and the relaxation time of the different transition states we calculated the internal friction of pure amorphous silica and mixed oxides.