

Mechanical Loss in Amorphous Pure and Doped Silica

Rashid Hamdan, Jonathan P. Trinastic, and H. P. Cheng *

*Department of Physics and Quantum Theory Project,
University of Florida, Gainesville, Florida 32611, USA*

The mechanical dissipation in the oxide coatings of many precision measurement systems is a major source of thermal noise that limits the performance of such devices. A good candidate for a coating material to reduce the mechanical loss is tantala (Ta_2O_5) doped with titania (TiO_2). Here, we numerically calculate the mechanical loss (internal friction) in these and other promising oxides based on the double well model. Using classical, atomistic molecular dynamics simulations, we estimate the density of double wells in the energy landscape of the amorphous oxides and the distribution of barrier heights, in addition to the deformation potentials, the elastic constants and vibrational frequencies at both the bottom of the potential wells and at the saddle points, all of which are relevant to the internal friction calculation. We use two versions of the bisection method to find the double well densities and distributions. All methods used in these calculations are implemented in DL-POLY molecular dynamics simulation software. These calculations will provide experimentalists with a better guide into which material combinations might be a better choice for reducing the mechanical loss.

* corresponding author: cheng@qtp.ufl.edu