

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Atomistic Modeling of Mechanical Loss in Pure and Doped Amorphous Oxides JONATHAN TRINASTIC, RASHID HAMDAN, HAI-PING CHENG, Dept of Phys. Quantum Theory Project, University of Florida — 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 tantalum (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.

rashid hamdan
Dept of Phys. Quantum Theory Project, University of Florida,

Date submitted: 15 Nov 2013

Electronic form version 1.4