Construction of Interatomic Potentials and Mechanical Loss in Nb_2O_5

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A BKS-Morse empirical potential is constructed for the *B* and *H* phases of Niobium Pentoxide (Nb_2O_5) for molecular dynamics simulation and energy landscape characterizations. Parameters of the interatomic potentials were adjusted to reproduce elastic properties of the two phases of Nb_2O_5 simultaneously. Given the absence of experimental data, we compared these elastic properties to those obtained using density function theory (DFT) calculations. We applied the potential to study amorphous Nb_2O_5 with structures generated by melting-quench classical molecular dynamics (MD) simulations. We then systematically located energy barriers for two-level systems. The energy barrier distribution collected from ~10^4 barriers can be compared to experiments. We use the distribution function and calculated relaxation time, mechanical coupling constants, etc. to obtain the mechanical loss (Q^{-1}), which is of importance to optical coating materials for the future generation of gravitational wave detection.