Mechanical loss in doped amorphous oxides with machine learning potentials

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Doped amorphous oxides (TiO_2-doped Ta_2O_5) providing very good optical and mechanical properties are used as mirror coatings in the Laser Interferometer Gravitational-Wave Observatory (LIGO) detector. To increase sensitivity, it is desirable to reduce the noise in the coatings. In this work we focus on thermal noise manifested by mechanical loss. Modeling doped amorphous oxides is extremely difficult due to their complicated energy landscape. Determining some properties requires a large simulation box to capture a fair sample of configurations. Hence fast and accurate potentials (or force field) are essential. We develop machine learning potentials based on spectral neighbor analysis (SNAP) for doped amorphous systems (ZrO_2-doped Ta_2O_5, TiO_2-doped GeO_2). Mechanical spectroscopy is used to simulate the stress responses from applied strains, which allows us to calculate the mechanical loss Q^{-1} from molecular dynamics (MD) simulations. The calculated mechanical losses increase as the temperature increases at high frequencies (> 10^9Hz). At 1kHz, the low-frequency power-law extrapolation Q^{-1} is 4×10^{-3} at 300K and 5×10^{-4} at 50K for 50% ZrO_2-doped Ta_2O_5. The mechanical loss dependence of the doping is also studied to find the optimal dopant and doping concentration.

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