An atomistic description of two-level systems and mechanical loss in tantala and titania-doped tantala

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The mechanical loss (Q^{-1}) intrinsic to amorphous oxides is the limiting factor for sensitive, high-precision gravitational wave detectors and optical devices. Recent experimental work indicates that doping amorphous tantala with titania reduces Q^{-1}, however the physical processes underlying this reduction are unknown. Here we calculate Q^{-1} for pure and titania-doped tantala using numerical methods combined with molecular dynamics simulations taking advantage of atomic levels of resolution. Our results show that 62-76 percent Ti doping minimizes the magnitude of the characteristic low-temperature loss peak, matching previous experimental results. We provide a microscopic explanation of this minimized loss by exploring how doping affects the potential energy landscape, strain coupling constant, elastic modulus, relaxation time, and other properties described within a double-well potential model. Finally, we compare configurational changes for characteristic two-level transitions to provide the first atomic description of loss behavior in these oxides. These results highlight the most important parameters dictating Q^{-1} in these mateirals and guide future screening of doping combinations to minimize mechanical loss.