Mechanical Loss and Raman Calculation of Germanium Dioxide

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Minimizing mechanical loss in LIGO's mirror coating materials is crucial for increasing measurement accuracy. A promising candidate to replace titania-doped tantala in current mirror coatings is titania-doped germania. In this work, we simulate the mechanical loss of pure germania using the two-level system (TLS) model. We use models made of 1008 and 2016 atoms to collect TLSs that contribute to mechanical loss at different temperatures and show that larger atomic structures can better simulate higher temperature loss. In conjunction, Raman calculations are applied to amorphous Germania structures as Raman spectroscopy is sensitive to the local vibrations of short and medium range order structures found in glasses. Performing Raman calculations on large structures, necessary for amorphous models, can be very time consuming and computationally expensive. Here, we introduce a novel method that drastically speeds up the calculation time while yielding results in good agreement with both experimental data and the conventional method.