Molecular dynamics modeling of amorphous tantala, titania, and silicates based on silica BKS potential

JP Trinastic[1], R Hamdan[1], YN Wu[1], HP Cheng[1]

[1]Department of Physics, Quantum Theory Project, University of Florida, Gainesville, FL 32611

Tantala and various silicates are important materials for medical applications due to their corrosion resistance and biocompatibility (Matsuno et al 2001, *Biomaterials,*22:1253), and both tantala and titania are central to reducing mechanical loss in mirror coatings used in the LIGO project (Harry et al 2007, *Class Quantum Grav*, 24:405). However, no molecular dynamics potentials have been created to date that combine tantala, silica, and other oxides that would allow important computational analyses to better understand the structural and mechanical properties of these materials with different dopants. To this end, we have created several interatomic potentials modeling van der Waals and covalent interactions that reproduce both the structure and mechanical properties of crystalline and amorphous tantala, titania, and hafnia. In addition, we have created the potentials so they can be used together and in conjunction with the robust BKS silica potential to allow the study of doping effects. Structural and mechanical properties are reported for crystalline and amorphous structures with various doping levels that match experimental data and results from density functional theory (DFT) calculations. Future analyses using these potentials will be of great value to determine optimal doping concentrations and material combinations for myriad material science applications.