Joint 20th AIRAPT – 43th EHPRG, June 27 – July 1, Karlsruhe/Germany 2005

Thermoelasticity at High Temperatures and Pressures: Molybdenum and Tantalum

Daniel Orlikowski, Randolf Q. Hood, Per Soderlind, and John A. Moriarty

Lawrence Livermore National Laboratory,

Livermore, CA 94551-0808, orlikowski1@llnl.gov

In an effort to develop multi-phase constitutive strength models that extend with some certainty beyond the thermodynamic regimes of experiments, two quantum-based methods that calculate either anharmonic or quasi-harmonic effects to elastic moduli have been developed for temperatures up to 26,000 K and for pressures up to 10 Mbar. In either approach, both the electron-thermal and ion- thermal contributions are combined to compose the elastic moduli. The full potential linear muffin-tin orbital(FP-LMTO) method for the cold and electron-thermal contributions is closely coupled with ion-thermal contributions. For the ion contribution two separate approaches are used. In one approach, the quasi-harmonic ion contribution is obtained through a Brillouin zone sum of the strain derivatives of the phonons, and in the other the anharmonic ion contribution is obtained directly through Monte Carlo (MC) canonical distribution averages of strain derivatives on the multi-ion potential itself. Both methods for the ion-contribution use many-body, quantum-based interatomic potentials derived from model generalized pseudopotential theory (MGPT). The resulting elastic moduli compare well to available ultrasonic measurements and diamond-anvil-cell compression experiments, as well as to sound speeds along the Hugoniot. Over this range of temperature and pressure, the results are used in a polycrystalline averaging for a comparison to large-scale constitutive models like the Steinberg-Guinan strength model. Both molybdenum and tantalum elastic moduli are compared for varying anharmonic effects.

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under contract W-7405-Eng-48.