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Anharmonic Materials and Thermoelasticity at High Temperatures and Pressures DANIEL ORLIKOWSKI, RANDOLF Q. HOOD, PER SODERLIND, JOHN A. MORIARTY, LLNL, Livermore, Ca 94551 — For large-scale constitutive strength models, the shear modulus is typically assumed to be linearly dependent on temperature. However, for materials compressed along or beyond the Hugoniot into high pressure and temperature regimes where there is no experimental measurement or very little, accurate and validated models must be used. To this end, we have investigated and compared, as a function of temperature (<26,000 K) and pressure (<10 Mbar), the anharmonic and quasi-harmonic thermoelasticity accounting for both the electron-thermal and ion-thermal contributions for bcc tantalum and bcc molybdenum. In this approach, 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 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 quantum-based interatomic potentials derived from model generalized pseudopotential theory (MGPT). The resulting elastic moduli are compared 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 then used in a polycrystalline averaging for a comparison to larger-scale shear models like the Steinberg-Guinan strength model. These results give an indication that anharmonic effects are negligible in tantalum but not in molybdenum for high pressures and temperatures up to melt. 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.

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