Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

High pressure thermoelasticity of vanadium[1] DANIEL ORLIKOWSKI, LLNL — To support a larger effort for a multi-phase constitutive strength model for vanadium, we discuss the calculations performed to determine the anharmonic thermoelasticity for bcc and rhombohedral phases of vanadium. In this investigation, we have performed extensive calculations of the elastic moduli over broad ranges of temperature (<10,000 K) and pressure (<3 Mbar), accounting for both the electron-thermal and ion-thermal contributions. Using density functional theory (DFT) with the projector augmented-wave (PAW) methodology to calculate the electron-thermal component, we have combined this with the ion-thermal component, which is calculated from Monte Carlo (MC) canonical distribution averages of the strain derivatives on a multi-ion potential itself. The ion-potential is described through a many-body, quantum-based interatomic potential—the model generalized pseudopotential theory (MGPT). We suggest regions of stability for the rhombohedral structure in the phase diagram. The resulting elastic moduli are compared to available experimental results and to sound speeds measured along the Hugoniot.

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Date submitted: 16 Dec 2008 Electronic form version 1.4