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High pressure lattice dynamics and elasticity of transition metals DANIEL ORLIKOWSKI, LORIN BENEDICT, JOHN KLEPEIS, Lawrence Livermore National Laboratory — For continuum-level description of transition metals using equation of state and strength models, a large concerted calculation effort is required. We present here a subset of that work to provide Debye temperatures and elastic moduli for the equation of state (EOS) and strength models. DFT calculations for the phonons are performed to obtain the Debye temperature over the pressure range required by the EOS model. For the strength model, we have combined several sets of quantum-based, atomistic calculations with density functional theory (DFT) to develop elastic moduli over a wide range of temperatures (12,000 K) and pressures (4 Mbar). Our focus is upon vanadium but other transition metals will be presented tantalum and molybdenum. Our results are comparable to available experimental data. 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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