High temperature and high pressure equation of state of gold

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Recent advances in high-pressure experimental technology have made it possible to obtain reliable measured data at extreme pressure conditions exceed 400 GPa. One of the most serious problems at present is how to accurately estimate the pressure conditions where measurements are performed. For example, discrepancies between the proposed Au pressure scales(Jamieson et al., 1982; Anderson et al., 1989; Shim et al., 2002; Dewaele et al., 2004) reach 12 GPa at 100 GPa and 20 GPa at 150 GPa even at room temperature. The aim of this study is to develop an accurate temperature-pressure-volume equation of state (T-P-V EOS) of Au without any pressure scale. Here we derive the T-P-V EOS of Au based on measured volume thermal expansion data up to 1300 K at 0 GPa(Nix et al., 1941; Suh et al., 1988), observed temperature dependence of bulk modulus at 0 GPa by ultrasonic sound velocity measurements(Collard and McLellan, 1991), and shock compression data up to 240 GPa(Marsh, 1980; Yokoo et al., 2008).

We estimate the lattice thermal pressures of Au at high temperatures based on the Mie-Gruneisen relation with the Debye thermal model and the Vinet isothermal EOS. The contribution of electronic thermal pressure at high T, estimated previously by Tsuchiya and Kawamura(2002) based on first-principles electronic structure calculations, was also included in this study. The Gruneisen constant is assumed to be independent of T, and the volume and the Debye temperature at 300 K and 0 GPa are fixed at 10.215 cm3/mol and 170 K, respectively from previous works(e.g. Heinz and Jeanloz, 1984). Using the measured data of Au as described above, we successfully optimized the four key EOS parameters of Au, namely the isothermal bulk modulus at 300 K, 0 GPa and its pressure derivative, and the Gruneisen constant at 300 K, 0 GPa and its volume dependence.

Simultaneous volume measurements of Au and MgO by synchrotron powder X-ray diffraction experiments have been made by Fei et al.(2004) using a Kawai-type multi-anvil high-pressure apparatus, and by Hirose et al.(2008) based on diamond anvil cell experiments. Here we estimated the pressures for these two X-ray experiments based on the Au EOS derived in this study and the MgO EOS developed previously by Matsui et al.(2000) using MD simulation. We found that, for both data by Fei et al. and Hirose et al., the Au pressures agree very well with the MgO pressures over wide T and P ranges, with the errors being within 0.6 GPa for 26 high T and P data up to 2173 K and 26 GPa by Fei et al., and within 1.9 GPa for 20 high T and P data up to 2080 K and 122 GPa by Hirose et al. Because both the present Au EOS and the MgO EOS by Matsui et al. were obtained using completely different techniques and without any pressure scale, the excellent consistency between the Au and MgO EOSs lends us much credibility in the two pressure scales at high temperatures and high pressures.