Comparison between the Au and MgO pressure scales at high temperature and high pressure

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The equation of state (EOS) of Au, proposed by Anderson et al.(1989), has recently been widely used to estimate pressure at high temperatures. Anderson et al. derived the EOS of Au based on the measured elastic and thermodynamic properties of Au at temperatures less than 550 K. On the other hand, Jamieson et al.(1982) obtained another Au EOS based on shock compression (high temperature and high pressure) data of Au. We note the difference in the estimated pressures between the two EOS's (P by Anderson et al. minus P by Jamieson et al.) reaches -2.5 GPa at 1500 K and 25 GPa.

As an alternative pressure scale of Au, Matsui et al.(2000) have recently developed a precise EOS of MgO at high temperatures and high pressures up to 3000 K and 100 GPa. They have derived the EOS of MgO using the Molecular dynamics (MD) simulation, thus taking fully account of anharmonicity at high temperatures.

Using a non-empirical Variational Induced Breathing (VIB) model and the MD method, Inbar and Cohen(1995) calculated the EOS of MgO at temperatures up to 3000 K and pressures up to 310 GPa, and found the computed bulk modulus and volume thermal expansivity of MgO, and their temperature and pressure dependencies agree very well with experiments.

We first compared the two MgO pressure scales developed based on the empirical(Matsui) and the non-empirical(Inbar and Cohen) interatomic potentials, to check the accuracy of the reported MgO presssure scales at high temperatures. We found excellent agreement between the two independent pressure scales over wide temperature and pressure ranges, with simulated pressure discrepancies between the two for specified relative volumes being within 0.5 GPa in the temperature and pressure ranges up to 2000 K and 30 GPa. Such excellent agreement between the two MgO pressure scales lends us much credivility in the T-P-V EOS of MgO proposed by Matsui(2000).

Nishiyama et al.(2001) have made in situ X-ray diffraction experiments for pyrolite at high temperatures and high pressures with a multi-anvil apparatus (SPEED-1500) at SPring-8, in which both Au and MgO were placed in the sample chamber to measure pressure. Here we compare estimated pressures based on the MgO scale(Matsui) with those based on the Anderson's Au scale, with the results that the Andrerson's Au scale underestimates pressures by 1.4 GPa relative to the MgO scale at 1873 K and around 20 GPa.