Pressure Calibration Standard at high Temperature and high Pressure

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In high temperature and high pressure experiments, it is crucial to have a reliable pressure calibration standard over wide temperature and pressure ranges. At room temperature, the ruby-fluorescence pressure scale is found to accurate to within 1 % up to 55 GPa(Zha et al., 2000). However, severe discrepancies are reported between proposed pressure scales at high temperatures.

We showed previously (Matsui et al., 2000) that by combining the molecular dynamics(MD) method with quantum correction, it is possible to simulate very accurately the structural and physical properties of crystals over wide temperature and pressure ranges. Since the MD method derives thermal properties directly without any constraint on the atomic displacements, it is particularly useful and powerful for the simulation at high temperatures where anharmonic effects are important. In order to take into account the many-body forces in crystals, the breathing shell model(BSM) developed by Matsui(1998) is used for the MD simulation.

We have applied the MD method to the four cubic crystals, MgO, NaCl, Ar, and γ-Mg_2SiO_4. We show the MD simulation with BSM reproduces very accurately the observed properties of these crystals, including the volume compression data at room temperature, the volume thermal expansion data at 0 GPa, and the elastic constants and their temperature and pressure dependences. We then simulate and crosscheck the *T-P-V* equations of state of these crystals to provide them as reliable internal pressure calibration standards at high temperatures and high pressures.

Keywords: MD simulation, pressure standard, high temperature