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Constraining the equation of state of fluid H₂O to 80 GPa using the MgO-H₂O system.

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Beamline: X17C

Introduction: The physical properties of H₂O are important geologically over a large range of pressure and temperature. Shock-wave data have served as the main resource for the derivations of many equations of state for fluid H₂O [1-3]. Direct measurements of the molar volume of water are required to test the validity of these models, however, these measurements are difficult and, as a result, rare. The study presented here sought to determine the *PVT* properties of Ice VII at pressures > 20 GPa and especially along the melting curve at high-pressures to further constrain the equation of state of fluid H₂O and to test the models of previous workers derived from low-pressure data and extrapolated to high-pressures.

Methods and Materials: A Mao-Bell type diamond anvil cell with an external heater was used in this study. The temperature of the experiment was determined by placing a type-S thermocouple (Pt-Pt_{0.9}Rh_{0.1}) between the diamond anvil and Re-gasket, directly against the surface of the diamond. Temperatures were kept constant to ±5 K during data collection, whereas the uncertainty associated with the thermocouple itself is ±2 K over the range of temperatures in this study. The diffraction pattern of H₂O, MgO and gold were monitored during the experiment. The unit cell of gold determined from the diffraction lines was used in conjunction with a previously established *PVT* equation of state [4] so that gold acted as an internal pressure calibrant. The 111, 200 and 220 diffraction lines of gold and 110 line of Ice VII were present in most analyses.

Results: Generally, experiments would follow the following sequence as temperature was increased: 1.) slight drop in pressure, 2.) the appearance of diffraction lines indicative of brucite, and 3.) total disappearance of Ice VII diffraction lines and noticeable drop in pressure (up to ~2 GPa at the highest pressures). The appearance of brucite would always proceed the disappearance of Ice VII diffraction lines. The data suggest that brucite formed from MgO as soon as fluid H₂O became available whereas Ice VII melted over a small range over temperature (>50 K). These results were used further to constrain the *PVT* properties of water at elevated pressures and temperatures by taking the pressure derivative of the Gibbs Free Energy difference between Ice VII and fluid H₂O along the Ice VII melting curve. The previously stated equations of state of fluid H₂O overestimate the molar volume of water at pressures > 35 GPa.

Conclusions: The study presented here sought to constrain the equation of state of fluid H₂O using the MgO-H₂O system along the Ice VII melting curve at pressures > 20 GPa using the a Mao-Bell type diamond anvil cell with an external Mo-wire resistance heater. The experiments were conducted on beam line X17C at the Brookhaven National Synchrotron Light Source using the Energy Dispersive X-ray Diffraction (EDXD) technique. These results will be used further to constrain the *PVT* properties of water at elevated pressures and temperatures by taking the pressure derivative of the Gibbs Free Energy difference between Ice VII and fluid H₂O along the Ice VII melting curve. Comparison of these results suggests that the previously stated equations of state of fluid H₂O underestimate the molar density of fluid H₂O at pressures > 35 GPa.

References:

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