Phase Relations and Melting Curve of Water at Extreme Conditions

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Properties and phase relations of ice and fluid water at high pressures and temperatures are of fundamental interest and important for a number of physical, chemical, geophysical, and technological problems. Information on fluid water at very high pressure and temperature has been obtained largely from shock-wave experiments. Ice VII is a stable water phase at room temperature above 2.3 GPa. The melting curve of ice VII was determined to 20 GPa by means of the pinhole technique of resistance measurement in the simple squeezer high-pressure and high-temperature devices. Melting relations were confirmed by Mishima and Endo (1978), who carried out the experiments with a multianvil pressure device. Later Fei et al. (1993) studied melting of ice VII to about 16 GPa by monitoring the disappearance of the (110) peak in the X-ray diffraction collected with energy dispersive detector. Datchi et al. (2000) based on visual observations of melting of water at pressure up to 13 GPa (temperatures about 750 K) found large discrepancies with respect to previous determinations at temperatures higher than 550 K. At 700 K the melting pressure differs in works of Fei et al. (1993) and Datchi et al. (2000) by 4 GPa. Resolving such a controversy requires further experimental studies with accurate *in situ* measurements of pressure and temperatures in diamond anvil cells.

We developed an external heating assembly which allows conducting experiments in DAC at pressures above 130 GPa and temperatures above 1200 K. It consists of external resistive heaters placed around a cell, temperature resistant loading system, and a miniature DAC of a cylindrical shape (diameter 23 mm, height 15 mm) made out of a special high-temperature Ti-based alloy. The new system allows fine (within 1 GPa) adjustment of pressure in the whole temperature range. It maintains constant pressure (within 1 GPa at megabar pressure range) and temperature (within 5 K at 1000 K) during several hours, allows measuring temperatures accurately with an external thermocouple, and does not have measurable temperature gradient within the pressure chamber.

The melting curve of ice VII was measured to maximum pressure of 50 GPa (temperature of about 1200 K). Experiments were carried out in an externally heated diamond anvil cell and melting was monitored by disappearance of X-ray diffraction from ice VII and by changes in Raman spectra. The melting line of H_2O was found to be well described by the Simon equation $P = 2.2 + 1.31\left[\left(T/365\right)^{3.3} - 1\right]$.