Raman spectra of diamond at high pressures and high temperatures

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It is known that diamond is optically transparent and the hardest material. The development of the diamond anvil cell (DAC) technique using these features has advanced Raman spectroscopy investigations of vibrational modes in materials at extreme high-pressure conditions. In such high pressures and high temperatures, the equations of state of reference materials, such as gold, platinum, and sodium chloride, have usually been used for the precise determination of the sample pressure. However, it is difficult to use the synchrotron X-ray diffraction technique in laboratory-based experiments. Although the fluorescence of ruby has been commonly used as the pressure sensor, it is impracticable at high temperatures. Thus, other optical pressure sensors have been proposed. It is known that the first-order Raman mode of diamond anvil has been considered as a strong candidate because its Raman signal is intense and the diamond is always used as the anvil material in the DAC experiments.

Gold powder, which was mixed with NaCl powder, was used as the pressure reference. The sample was probed using angle-dispersive X-ray diffraction, located at the synchrotron beam line, at the BL10XU of SPring-8 (Japan). The pressure was determined from the unit cell volume of gold using the equation of state for gold. The unpolarized Raman spectra of diamond were acquired using a Raman spectrometer system, which was installed in the synchrotron beamline.

The shift in frequency of the first-order Raman band of diamond with changing pressure and temperature was investigated to 800 K and 106 GPa [1]. The pressure dependence is nearly linear at pressures below 40 GPa. However, deviation of the pressure dependence from the linear equation has been confirmed at higher pressures. The frequency decreases with increasing temperature at ambient pressure. The temperature dependence is small with an increasing pressure, as determined from experiments conducted along isotherms up to 106 GPa. The relationship between the shift of this band and temperature can be described by a polynomial equation [1]. Therefore, this pressure sensor has the advantage that it is not necessary to mix any additional calibration materials with the samples in the DAC experiments.

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