Cubic boron nitride under extreme conditions of high pressure and temperature: a combined Raman and theoretical study

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Cubic boron nitride (cBN) has several remarkable properties including extreme hardness, chemical inertness, high thermal conductivity, and a wide band gap, that makes it attractive for many practical applications including abrasives, protective coating and microelectronic devices. Since most of these properties include the use of the material at extreme conditions, the study of its physical properties under these conditions is essential.

It has been suggested [1], that cBN can be used as a pressure sensor because of the stability of its crystal structure under very high pressure. Use of cBN as a Raman pressure gauge at simultaneous conditions of high pressure and temperature has been proposed recently [2-4], but the corresponding experimental studies are limited to 1550 K at approximately 9 GPa [2] and 727 K at 20 GPa [3]. No theoretical calculations of the vibrational properties *c*BN at simultaneous high pressure and temperature are reported.

In this work, Raman spectroscopy in the diamond anvil cell and density functional calculations have been used to determine the pressure dependence of the transverse zone-center optical phonon mode to 40 GPa and 2000 K. High temperatures were achieved using laser heating combined in some cases with internal (resistive) heating. Powdered alumina and argon served as pressure media. The results establish a high-pressure scale at high temperatures based on the measured and calculated frequency of the transverse optical mode. Our experiments show that cBN can be conveniently used as in situ pressure sensor to at least 2400 K and 40 GPa.

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