Structure and Raman frequency of 3C-SiC under nonhydrostatic stress

LEI LIU[1], LI YI[1], HONG LIU[1], LONG-XING YANG[1]

[1] Key Laboratory of Earthquake Prediction, Institute of Earthquake Science, China Earthquake Administration, Beijing, China. liulei@cea-ies.ac.cn

Diamond anvil cells (DACs) have long been extensively used to generate high pressure on materials for research purposes (Dubrovinsky et al., 2015). However, maintaining hydrostatic conditions under such extreme pressures has long been a great challenge. At extreme pressures, pressure induced solidification of the PTM is inevitable and effects of non-hydrostatic stress caused by PTM solidification will become more and more ineligible with increasing pressure. The stress in the PTM and the sample will both begin to depart from hydrostatic under extreme pressures.

Nonhydrostatic stress has been reported to have unique influence on material. First-principles simulation methods are more suitable for this job (Gillan et al. 2006; Wentzcovitch and Stixrude, 2010; Jahn and Kowalski 2014)by calculating the properties of materials, such as the state of nonhydrostatic (differential) stress and its effects at atomic scale (Parrinello and Rahman 1982; Liu et al. 2014, 2016). For understanding the quantitative effect of nonhydrostatic stress on properties of material, the crystal structure and Raman spectra of 3C-SiC under hydrostatic and nonhydrostatic stress were calculated using a first-principles method. The results show that the lattice constants under nonhydrostatic stresses deviate those under hydrostatic stress. The differences of the lattice constants (***a, b*** and ***c***) under hydrostatic and nonhydrostatic stresses with differential stress were fitted by linear equation. Nonhydrostatic stress has no effect on density of 3C-SiC at high pressure, namely the equations of state of 3C-SiC under hydrostatic stress are same as those under nonhydrostatic stress. The frequencies and pressure dependences of LO and TO modes of 3C-SiC Raman spectra under nonhydrostatic stress are just same as those under hydrostatic stress. Under nonhydrostatic stress, there are four new lines with 361, 620, 740, and 803 cm-1 appeared in the Raman spectra except for the LO and TO lines because of the reduction of structure symmetry. However the frequencies and pressure dependences of the four Raman modes remain unchanged under different nonhydrostatic stresses. Appearance of new Raman modes under nonhydrostatic stress and the linear relationship of the differences of lattice constants under hydrostatic and nonhydrostatic stresses with differential stress can be used to indicate state of stress. The effect of nonhydrostatic stress on materials under high pressure is very complicated and our calculation would help to understanding state of stress at high pressure experiments.