Electronic Structure Changes in Anthracene Crystals under Static and Shock Compression: Role of Nonhydrostaticity

Zbigniew A. Dreger, Naoki Hemmi, and Yogendra M. Gupta
Institute for Shock Physics, Washington State University, Pullman, WA 99164-2816, USA

High pressure response of molecular crystals is not as well understood as the response of covalent or ionic crystals. Because molecular crystals are highly compressible, small variations in applied stresses result in large intermolecular changes. In addition, because of low symmetries resulting deformations, high pressure effects in these crystals are sensitive to nonhydrostaticity.

To understand the role of nonhydrostaticity on electronic structure changes in molecular solids, we examined anthracene crystals up to ~ 8 GPa under various loading conditions. The fluorescence and absorption experiments were performed to characterize differences in electronic structure of anthracene crystals under hydrostatic and nonhydrostatic (static and shock) compression. Under hydrostatic loading the changes in absorption and fluorescence spectra were gradual and reversible, and only red shifts are observed. In contrast, the onset of non-hydrostatic conditions generates several new features: (i) emergence of a new absorption band, (ii) deviation in absorption and fluorescence peak shifts, (iii) broadening of vibrational peaks, and (iv) occurrence of fluorescence with the excimer-like characteristics.

The spectroscopic results indicate the formation of new electronic states under nonhydrostatic conditions as a consequence of high stress and plastic deformation. The origin of new states is discussed and attributed to dimer-type defects formed in nonhydrostatically compressed (statically or shocked) anthracene.

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