Application of high-pressure spectroscopy to identify the UV color center in 2D boron nitride

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Abstract

Layered boron nitride is one of the key two-dimensional (2D) materials and is the subject of intensive research, both due to numerous new physical phenomena and advanced applications. It comprises boron and nitrogen ions forming flat sp^2 covalent bonds with a honeycomb structure inside the layers and weak van der Waals bonds between the layers, creating a three-dimensional crystal with a wide indirect bandgap of ~6 eV [1]. This bandgap accommodates numerous optically active electronic states of structural defects and impurities that are abundant in currently grown crystals and epitaxial layers. They can act as bright single photon sources with various photon energies or as efficient light emitters with extreme thermal stability [2-5]. One of the brightest emissions at ~4 eV originates most likely from a carbon dimer-related defect [3,4,6,7]. To fully control and develop unique BN applications on demand, both the nature and electronic structure of color centers should be identified.

The most common 2D BN is centrosymmetric hexagonal BN (hBN), but the BN atomic planes can also be arranged in non-centrosymmetric configurations like rhombohedral (rBN) or Bernal (bBN). Different layer stacking sequences influence the UV emission of color centers in the BN host [7]. In this work, we used the diamond anvil cell technique to perform high hydrostatic pressure studies of the low-temperature photoluminescence (PL) of hBN, rBN, and bBN in the 3 – 4.2 eV spectral region. The results showed that the PL energy (E_{PL}) decreased with pressure less sensitively than the bandgap, and the observed pressure coefficients of E_{PL} depend strongly on the BN polytype. Theoretical calculations of pressure dependencies of various defect levels in BN polytypes confirmed that the observed emission was associated with carbon-related defects. Our results show that tuning the stacking sequence in various polytypes of a given crystal provides unique “fingerprints” contributing to identifying defects in 2D materials [8].

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