

Identification of UV color center in 2D boron nitride - polytype control and high-pressure studies

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Layered boron nitride is a wide bandgap semiconductor, which in its hexagonal form (hBN) was already synthesized in the 19th century. However, only recently, high-quality single crystals with macroscopic size were produced, leading to the realization of a light-emitting device operating in the deep UV [1]. This achievement paved the way for applications of hBN in advanced optoelectronics, making it to be considered a challenger to aluminum nitride. Furthermore, in 2016, Bourrellier et al. reported single photon emission of a color center emitting at 4.1 eV [2]. The nature of the defect giving rise to this behavior has become the subject of intense research and discussion.

In order to contribute to the elucidation of the origin of such emission, we performed high hydrostatic pressure studies of the low-temperature photoluminescence of hBN crystals and other BN stacking sequences, i.e., the Bernal bBN) and rhomboedral (rBN) forms (polytypes) using the diamond anvil cell technique. The results showed that the emission energy decreased with pressure less sensitively than the bandgap [3,4]. This behavior is typical of deep traps. Theoretical calculations of pressure dependencies of various defect levels in hBN and other BN polytypes demonstrated that the observed emission is associated with carbon-related defects, and its pressure behavior depends on BN polytype. Our results show that tuning the stacking sequence provides unique “fingerprints” contributing to the identification of defects in 2D materials [5].

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