High-pressure study of UV emission of color centers in hexagonal boron nitride - experimental and theoretical analysis

A. Kaminska [1,2,3], K. Koronski [1], S. Li [4], A. Perhsin [4,5], A. Gali [4,5], J. Plo [6], A. Ibanez [6], P. Valvin [6], J. Li [7], T. Poirier [7], G. Cassabois [6], J. H. Edgar [7], and B. Gil [6]

[1] *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, PL-02668 Warsaw, Poland*
[2] *Faculty of Mathematics and Natural Sciences. School of Exact Sciences, Cardinal Stefan Wyszynski University, Dewajtis 5, PL-01815 Warsaw, Poland*
[3] *Institute of High Pressure Physics 'Unipress', Polish Academy of Sciences, Sokołowska 29/37, PL-01142 Warsaw, Poland*
[4] *HUN-REN Wigner Research Centre for Physics, P.O. Box 49, H-1525 Budapest, Hungary*
[5] *Department of Atomic Physics, Institute of Physics, Budapest University of Technology and Economics, Műegyetem rakpart 3., H-1111 Budapest, Hungary*
[6] *Laboratoire Charles Coulomb, UMR 5221, CNRS-Université de Montpellier, 34095, Montpellier, France*
[7] *Kansas State University, Tim Taylor Department of Chemical Engineering, 1005 Durland Hall, 1701A Platt St., Manhattan, KS 66506-5102*

Hexagonal boron nitride (hBN) is a wide bandgap semiconductor which was synthesized already in the 19th century, but only recently a high quality, single crystals with macroscopic millimetric size were produced [1], leading to the realization of a light-emitting device operating in the deep UV [2]. This achievement paved the way for applications of hBN to advanced optoelectronics, making it to be considered a challenger of aluminum nitride [3]. Furthermore, Bourrelier et al. reported in 2016 single photon emission of color centers emitting at 4.1 eV [4]. The question of the nature of the defect giving rise to this behavior is under debate.

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 bulk h-BN crystals in 3.3–4 eV spectral region using the diamond anvil cell technique. Our measurements revealed that the emission energy decreased with pressure less sensitively than the bandgap [5]. This behavior at variance from the shift of the bandgap is typical of deep traps. Interestingly, hydrostatic pressure reveals the existence of levels that vary differently under pressure (a smaller decrease of the emission energy compared to the rest of the levels in this energy region or even an increase of it) with pressure. Theoretical calculations of pressure dependencies of various defect levels in hBN revealed that some of the observed UV lines are associated with carbon-related defects, and their pressure behavior depends strongly on hBN polytype i.e., different layer stacking sequences. This discovery enriches the physics of the UV color centers in hBN.

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