Carbon dimer defect as the origin of the 4.1 eV luminescence in hexagonal boron nitride

Mažena Mackoit-Sinkevičienė[1], Marek Maciaszek[2], Chris G. Van de Walle[3], Audrius Alkauskas[1]

[1]*Center for Physical Sciences and Technology (FTMC), Vilnius LT-10257, Lithuania*

[2]*Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warszawa, Poland*

[3]*Materials Department, University of California, Santa Barbara, California 93106-5050, USA*

mazena.mackoit@ftmc.lt

Hexagonal boron nitride (hBN) has attracted considerable interest over the past decade as a versatile material that can be used in a number of applications due to its unique combination of physical and chemical properties. In as-grown samples bright luminescence with a clear zero-phonon line (ZPL) at 4.1 eV is often observed [1]. The emission is believed to be due to defects. The line can act as a source of single photons [2]. Despite a ubiquitous nature of the 4.1 eV emission, the chemical nature of the defect, which responsible for luminescence, has not been established, even though the involvement of carbon is often assumed [3].

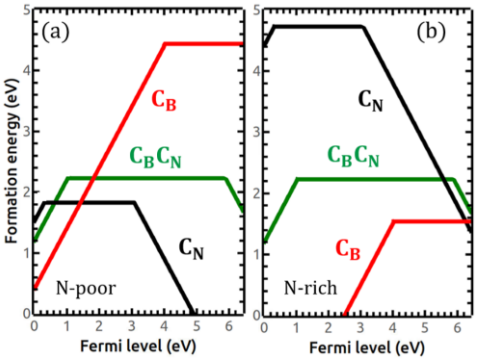

Fig. 1. Formation energy vs. Fermi level for C_B, C_N, and C_BC_N defects in various charge states under (a) N-poor and (b) N-rich conditions.

Based on hybrid functional first-principles calculations we propose that the neutral carbon dimer defect, C_BC_N, is responsible for the observed emission. We find that neutral C_BC_N is the most stable for Fermi levels throughout most of the band gap, with a formation energy of 2.2 eV. We find that there is a range of atomic chemical potentials and Fermi levels where the dimer is the most stable defect, indicating that it will form whenever carbon is present.

Carbon dimer accounts for all known experimental facts about the 4.1 eV luminescence: the involvement of carbon, the energy of the transition, the very short radiative lifetime, and moderate electron-phonon coupling. All these results allow us to propose the C_BC_N as a defect responsible for the 4.1 eV emission in hBN. In fact, carbon dimer defects have been indeed observed in transmission electron microscopy experiments on hBN [4].

REFERENCES

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