Point defects in hexagonal Boron Nitride

J. Strand[1] A. Shluger[1]

[1]Department oh Physics and Astronomy, University College London, Gower St, London, WC1E 6BT

Boron nitride is a promising candidate as a dielectric layer in 2D-material based devices [1]. Bulk hexagonal boron nitride (hBN) is isostructural to graphite, forming a layered honeycomb structure where boron and nitrogen atoms are held together by strong sp^2 bonds, giving hBN excellent mechanical strength and chemical stability [2,3]. Likewise, single layer hBN is also isostructural with graphene. Unlike graphene, however, single layer hBN is an insulator with a nonzero band gap between 5 and 6 eV [4].

In devices, semiconductor function is affected by the presence of intrinsic defects. For example, it is known that oxygen vacancies in semiconducting oxides (SiO_2, HfO_2) are linked to the filament formation process in resistive RAM devices [5,6]. Studies [7] have shown boron vacancies to be related to the analogous breakdown process in multilayer hBN.

Here we present the results of our investigation into hBN and a collection of its intrinsic defects. Using density functional theory (DFT), we analyse are range of defects in hBN, including boron and nitrogen vacancies, interstitials and Stone-Wells defects. We present the charge transition levels (CTLs), the ground state spin configuration, and the formation energies of the defects.

We use the CP2K software package [8] to implement DFT. This uses a Gaussian type atomic centred basis set and calculates electronic structure in the gamma point. We use a hybrid-DFT functional to calculate exchange and correlation energies. The calculations use 6x6x4 supercells in periodic boundary conditions. This particular cell expansion was used to give an effective K-point spacing which would sample the HOMO and LUMO states [9].

The CTLs of the intrinsic defects are calculated and, by alignment with typical electrode workfunctions, it is found that a number of intrinsic defects can be charged during device function. Divacancies are found to have positive binding energy. In particular, the formation of a "molecular bridge" in interlayer divacancies increases their stability. For example, in the lowest energy configuration of an interlayer boron divacancy, two N atoms form a N-N bridge across the layers. This greatly deforms the surrounding structure and reduces the energy required to form a boron vacancy-interstitial pair. The structure and dynamics of such defects may play a significant role in the breakdown of hBN in nanoelectronic devices.

[1] Dean, Cory R., et al., *Nature Nanotechnology* **5**, 722 (2010).
[2] Song, Li et al. , *Nano Letters* **10**, 3209 (2010).
[3] Chen, Ying, et al., *Applied Physics Letters* **84**, 2430 (2004).
[4] Watanabe, Kenji et al., *Nature Materials* **3**, 404 (2004).
[5] Padovani, A et al.et al, *Journal of Applied Physics* **121**, 155101 (2017).
[6] Bradley, S et al., *Physical Review Applied* **4**, 064008 (2015).
[7] Pan, Chengbin, et al, *Advanced Functional Materials* **27**, 1604811 (2017).
[8] VandeVondele, J, et al., *Computer Physics Communications* **167**, 103 (2005).
[9] Kharche N, et al. , *Nano Letters* **11**, 5274 (2011).