Energetics and Electronic Structures of Hexagonal Boron Nitride Thin Films with Monatomic Defects

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Hexagonal boron nitride (hBN) is a binary honeycomb sheet consisting of boron and nitrogen, which form bulk and thin film structures by stacking via weak interlayer interactions. According to weak interlayer interactions, hBN thin films can possess various metastable stacking morphologies that are energetically degenerate. Some of those thin films exhibit an electric dipole normal to the layers owing to the asymmetric interlayer atomic arrangement [1]. In addition to interlayer stacking, imperfections, such as atomic vacancies and substitutional defects, decisively affect the electronic structure of a hBN monolayer [2]. In the usual thin films, the interlayer stacking and the imperfections cooperatively affect their electronic properties. Thus, we investigate the electronic properties of hBN thin films with monatomic vacancies regarding the stacking arrangement and the defect position in the thin films, using density functional theory with generalized gradient approximation.
Here, we focus on 5-layer hBN thin films, one of which layers possesses monatomic vacancies with defect densities of $10^{13}/cm^2$ (Fig. 1). Our calculations show that the total energies of hBN thin films with monatomic vacancies are sensitive to defect species and location in the thin films. Electronic structures of the hBN thin films with monatomic vacancies are also sensitive to defect species, location in the thin films, and stacking arrangements. The defects induce an electric polarity in hBN thin films regardless of stacking arrangement.

References

[1] M. Maruyama and S. Okada FlatChem 48 (2024) 110571.
[2] D. Kozawa et al. Nanotechnol. 34 (2023) 115702.

Figures

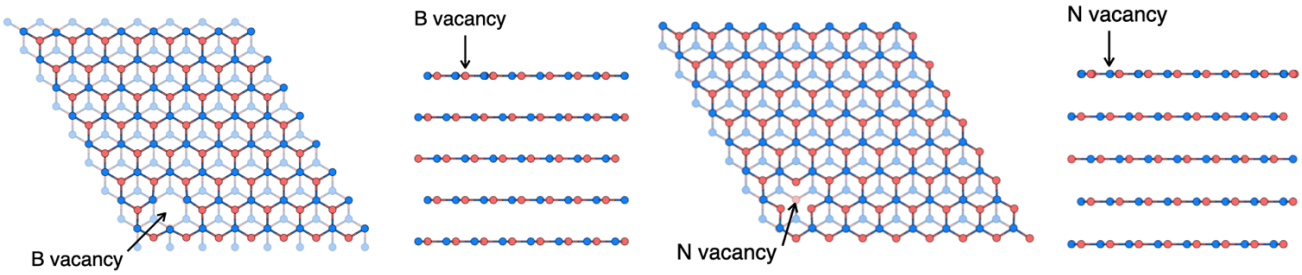

Figure 1: Geometric structures of hexagonal boron nitride thin films with monatomic vacancies in the outermost layer. Red and blue balls denote boron and nitride atoms, respectively.