Electrostatic properties of hexagonal boron nitride thin films

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Electronic structures of thin films consisting of atomic layer materials are sensitive to the constituent elements, their stacking arrangement, and the number of layers, even though the layers are bound via weak interlayer interaction [1,2]. In addition to the electronic structures, electrostatic properties of atomic layer materials are also sensitive to the interlayer stacking arrangement. It has been reported that hexagonal boron nitride (hBN) with AB (BA) stacking arrangement possesses ferroelectricity because of the finite polarization normal to the layers arisen from the symmetry breaking with respect to the stacking direction [3]. Because atomic layer materials have a lot of stacking variations, it is uncertain how the electrostatic properties of bilayer and thin films of atomic layer materials depend on their stacking arrangements. Therefore, in this work, we aim to investigate electrostatic properties of hBN thin films in terms of their stacking arrangements by using density functional theory combined with effective screening medium method.
Our calculations show that electrostatic potential difference between the upper and lower hBN layers is sensitive to the stacking arrangements. Bilayer hBN with AB (BA) stacking arrangement has the polarization normal to the layers causing the potential difference of 0.12 V between the layers. The polarization monotonically decreases with increasing the interlayer dislodgement along an armchair direction (Δ). The polarization vanishes at Δ = 0.83 Å and changes its direction at Δ = 1.24 Å (Fig. 1). We also found that the electrostatic potential across the layer also depends on the number of layers.

References

[1] M. Koshino, Phys. Rev. B, 81 (2010) 125304.
[2] Y. Gao and S. Okada, Appl. Phys. Express, 16 (2023) 075004.
[3] K. Yasuda et al. Science, 372 (2021) 1458.

Figures

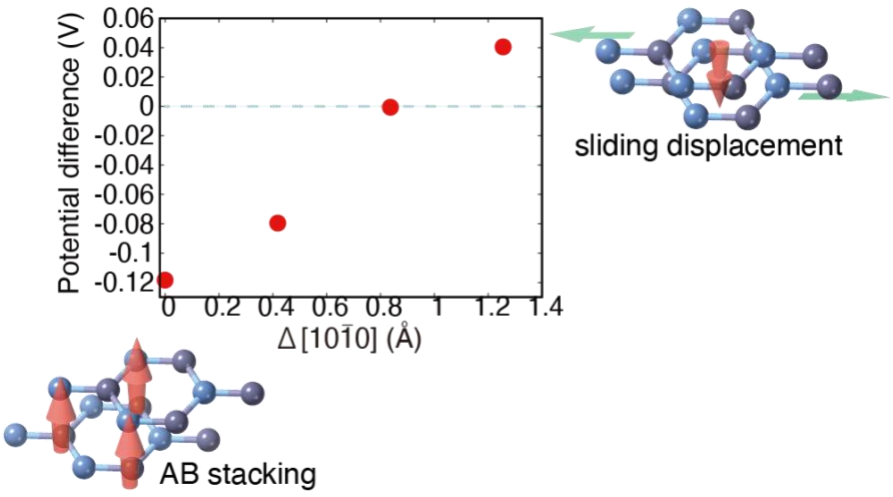

Figure 1: Potential difference of bilayer hBN between the upper and lower layers as a function of sliding displacement Δ in the armchair direction. Violet and blue balls denote B and N atoms, respectively.