Energetics of hexagonal boron nitride nanoflakes: Nucleation and growth processes of its bilayers

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In recent years, hexagonal boron nitride (h-BN) has emerged as a key supporting material in nanotechnology as insulating substrates and encapsulation layers for atomic-layer materials [1]. In addition to its practical applications, h-BN can exhibit various polymorphs in its bilayer and thin films, owing to weak van der Waals interactions [2]. Bilayer hBN with AA' and AB stacking arrangements are nearly degenerate in energy, with energy differences within a few meV per unit cell [3]. This fact raises a fundamental question: how is the stacking arrangement determined during the formation process? In this work, we aim to elucidate the energetics of hBN flakes and nucleation of the second hBN layer using density functional theory combined with the effective screening medium method. Fig. 1 shows that the formation energies of triangular h-BN flakes depend on the chemical potential of B and N atoms. On the hBN sheet, the flakes are bistable at or around the angles of 0˚ and 60˚, corresponding to AA' and AB stacking, respectively [Fig. 2]. We also demonstrated that the energy barriers for rotation increase with flake size, indicating that the stacking orientation of the hBN bilayer is determined during the early stages of nucleation.

References

[1] L. Wang, et al. Science **342** (2013) 614.
[2] K. Watanabe, T. Taniguchi, and H. Kanda, Nat. Mater. **3** (2004) 404.
[3] N. Marom, et al. Phys. Rev. Lett. **105** (2010) 046801.

Figures

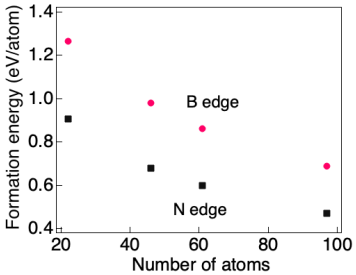

Figure 1: Formation energy per atom of triangular hBN nanoflakes with clean B and N edges as a function of the nanoflake sizes corresponding to the number of atoms. Circles and squares denote the energies of nanoflakes with N and B edges, respectively.

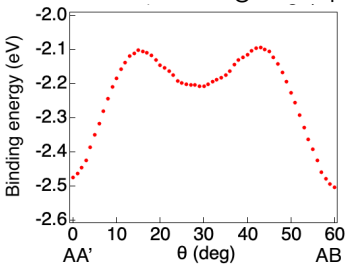

Figure 2: Total energy of [5]-hBN nanoflake with 12.5 Å boron edge on h-BN substrate as a function of orientation angle.