One-Dimensional Hexagonal Boron Nitride Semiconductor

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Hexagonal boron nitride (hBN), analogous to graphene, is a bi-elemental material comprising alternating boron and nitrogen atoms. Contrast to variable proposed applications of graphene electronic devices, however, applications of hBN in electronic device have been very limited only as a substrate for graphene-based nanodevices due to its insulating feature with a large band gap. In this presentation, we introduce one-dimensional semiconducting hBN channel using AA'/AB stacking boundaries of few-layer hBN grown by chemical vapor deposition (CVD).

We studied few-layer hBN grown on a Cu foil by CVD using transmission electron microscopy (TEM). Both AB-stacked hBN and AA'-stacked hBN were observed, and the boundaries between AA' and AB stacking were identified with atomic resolution. Atomically thin twin boundaries with a novel 6'6' configuration were revealed at AA'/AB stacking boundaries. The atomic configuration at the twin boundary are deeply analyzed whether it is 558 or 6'6' structure by combination of TEM simulation, density functional theory calculations and molecular dynamics simulations. Notably, the 6'6' configuration at stacking boundaries shows a semiconducting feature with a near-zero bandgap, which thus appears promising as a one-dimensional electron channel embedded in the original insulating hBN sheet. Furthermore, we propose the formation mechanism of twin boundaries by analogy with observations of extended Klein edges at the boundaries between a monolayer and bilayer in AB-stacked hBN. Atomically thin twin boundaries were created only when AA' and AB stacking merge in given stacking orientations, which will be explained in the presentation. This will give the insight for the controllable fabrication of single-hBN electronic devices.

References

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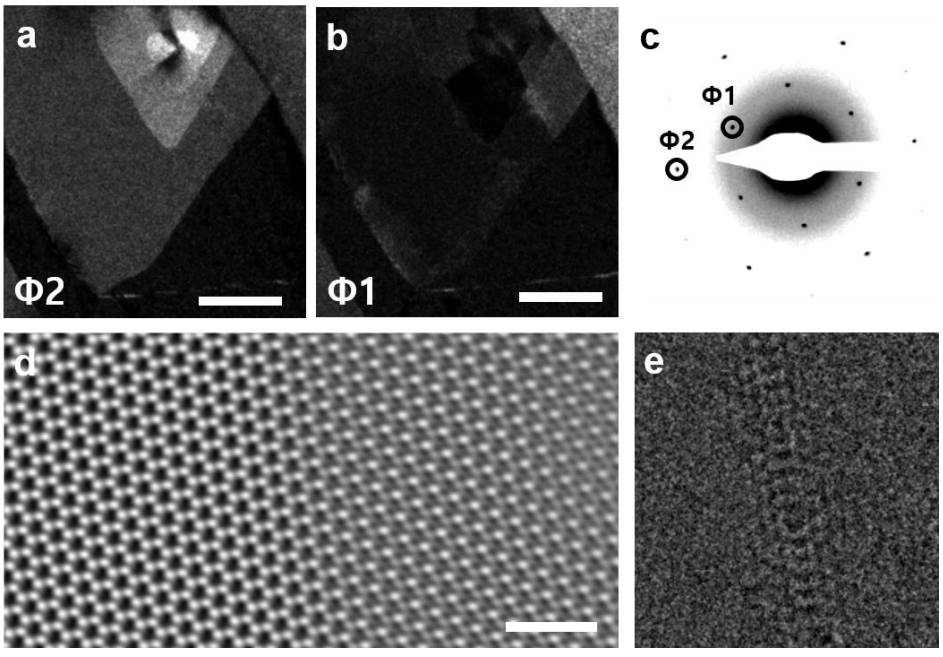

Figure 1. Atomically thin twin boundary in AA"- and AB-stacked hBN film. (a,b) Dark field TEM images of triangular, few-layer hBN islands from a second-order diffraction spot (Φ2), and a first-order diffraction spot (Φ1) displayed in (c). (d), HR-TEM image of the stacking boundary of a tri-layer ABA/AA"A-stacked hBN film.

(e) Fourier-filtered image obtained from the inverse of the power spectrum, after removing typical hBN lattice information, to extract the 6"6" configuration. Scale bar in (a,b), 0.1m and (c), 1nm.