Screw Dislocation-Driven Growth of Double-Helical Hexagonal Boron Nitride

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Hexagonal boron nitride (hBN), a two-dimensional (2D) layered material, shows enormous potential as a critical substrate in 2D heterostructured devices because of its atomically flat surface, unique insulating nature, and high stability. Numerous studies have used chemical vapor deposition to achieve the controllable and large-scale synthesis of hBN monolayer films for application in scalable electronic devices. However, understanding of its growth mechanism, especially for multilayers, is still lacking. Only few studies have discussed the growth process. In one of the first studies on monolayer hBN grown on Cu, Kim et al. reported that the growth was not self-limited and multilayer islands were observed after extended growth periods. They concluded that the growth mechanism changed to the Stranki - Krastanov model (island on layer) after the completion of the first layer. In contrast, based on the in-situ observation of Cu lattice expansion during hBN growth, Kidambi et al. proposed that multilayer hBN grows beneath the first layer in an inverted wedding cake structure formed by the incorporation of B atoms into bulk Cu. Herein, we show that multilayer hBN islands can be formed by screw dislocations at grain boundaries using transmission electron microscopy (TEM).

TEM study of multilayer hexagonal-shaped h-BN islands on a suspended monolayer film showed hexagonal spiral contours divided by a domain boundary. It is observed that an isolated multilayer island have double helical structures and more complex multilayer islands are merged with multiple screw-dislocations situated close together along domain boundary. A formation mechanism of hBN spiral was inferred based on TEM analysis as follows; First, the spiral starts from the domain boundary. When two domains in different orientation meet, B-B or N-N atoms face each other. Instead of stitching perfectly, each BN and NB domains climb one atom thick, where two screw-dislocations are initiated. And then grow forward across the domain boundary and keep grow in lateral direction. Once each spiral reaches domain boundary again, next layer are further grown on top of the other domain and keep growing in a same way. Unlike screw dislocation-based growth in nanoplates and other 2D materials (e.g., MoS2 and WS2) screw dislocations in hBN always appear as one pair because they initiate at domain boundary where two oriented domains with different polarities from the first layer.

References

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This work was supported by IBS-R019-D1.

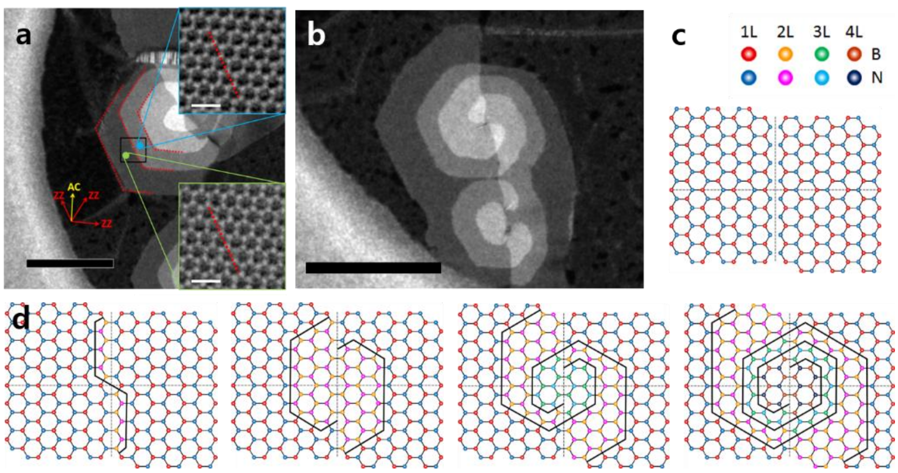

Figure 1. Double helical structure of few-layer hBN islands. (a) DF-TEM and HR-TEM image in few-layer a hBN island. (b) Double helix divided by domain boundary in DF-TEM image. (c) Atomic model of aligned hBN domain boundary. (d) Growth mechanism of hBN spirals. Scale bar in (a,b), 0.2m and (a) inset, 1nm.