Growth Mechanism of Hexagonal Boron Nitride: by Nanocrystalline Graphene Assistance and/or by B-N molecular diffusion

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Abstract

Hexagonal boron nitride (h-BN) has received a great deal of attention as a substrate material for high-performance graphene electronics because it has an atomically smooth surface, lattice constant similar to that of graphene, large optical phonon modes, and a large electrical band gap. Herein, we discuss

In the first part, we report the large scale synthesis of high-quality h-BN nanosheets in a chemical vapor deposition (CVD) process by controlling the surface morphologies of the copper (Cu) catalysts [1]. It was found that morphology control of the Cu foil is much critical for the formation of the pure h-BN nanosheets as well as the improvement of their crystallinity. We demonstrate the performance enhancement of CVD based graphene devices with large-scale h-BN nanosheets. The mobility of the graphene device on the h-BN nanosheets was increased 3 times compared to that without the h-BN nanosheets. The on-off ratio of the drain current is 2 times higher than that of the graphene device without h-BN.

We can determine occasionally nanocrystalline graphene (nc-G) on Cu foil during h-BN growth process. Unintentionally formed nanocrystalline graphene (nc-G) can act as a useful seed for the large-area synthesis of hexagonal boron nitride (h-BN) nanosheets with an atomically flat surface that is comparable to that of exfoliated single crystal h-BN. A wafer-scale dielectric h-BN nanosheets was successfully synthesized on a bare sapphire substrate by assistance of nc-G without metal catalyst [2]. We systematically discuss the growth mechanism of these nc-G-tailored h-BN nanosheets in the second part.

Until now, because of the low solubility of N atoms in metals, hexagonal boron nitride (h-BN) growth has explained by surface reaction on metal rather than by penetration/precipitation of B and N atoms in metal. In the third part, we present an impressive pathway of h-BN formation at the interface between Ni and oxide substrate based on B-N molecular diffusion into Ni through individual atomic vacancies [3]. First-principles calculations confirmed the formation energies of the h-BN layers on and under the metal and the probability of B-N molecular diffusion in metal. The interface growth behavior depends on the species of metal catalysts, and these simulation results well support experimental results.

These approaches provide a novel method for preparing high-quality two-dimensional materials on a large surface.

References

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Figures

a) nc-G growth on Cu foil / nc-G transfer on c-Al₂O₃ wafer / h-BN growth
b)