Domain shape engineering of CVD grown hexagonal boron nitride

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Hexagonal boron nitride (h-BN) also known as "white graphene" is a prominent member of the 2D materials family, which has gained a significant attention for its remarkable properties in the last decade. Its superior thermal conductivity (1700-2000W mK^{-1}), high mechanical strength (15.7 Nm^{-1}), large band gap energy (6 eV), atomically smooth surface, ultra-high flexibility, and transparency make h-BN a suitable candidate for numerous applications such as flexible and transparent electronics.

Owing to its binary element nature, the growth of high quality and large area CVD h-BN with controlled morphology is still a challenging task. CVD grown single crystalline h-BN domains exhibit various morphologies such as triangles, truncated triangles, hexagons, and other irregular shapes. Oftentimes edges of the triangular domains are nitrogen terminated while the hexagonal domains are having alternatively nitrogen and boron terminated zigzag edges[1]. Similarly, other shapes (polygon, circular and elliptical etc.) have their specific termination at the edges[5]. The morphology of h-BN domains has been found to depend on various parameters including surface roughness[1], growth temperature[2], water assisted argon to hydrogen ratio[3], position of the substrate[4], hydrogen passivation[5], substrate orientation[6] and the annealing time of the substrate[7].

In this work, we investigated the impact of precursor mass on the modification of the shape of h-BN domains. Synthesis of h-BN has been done by CVD process on polycrystalline copper foils using Ammonia Borane (AB) as a precursor. It is observed that the mass of the AB plays a key role in shape-influencing parameters of h-BN domains. With the increase in the weight of AB, h-BN growth is dominated by compact hexagonal domains whilst a decrease in the weight (<30 mg) leads to triangular and other irregular domains. We also observe that diluted hydrogen leads to the appearance of unusual elliptical and circular shapes.

Characterization of h-BN samples has been done by XPS, UV-Vis spectroscopy, Optical microscopy RAMAN, ToF-SIMS, and SEM. XPS data confirms that the binding energy of boron and nitrogen is around 190 eV and 398 eV, respectively, which are very close to the values reported in the literature. As grown h-BN on the top surface of the foil (directly exposed to precursor flow) and on the bottom surface (confined with the quartz support) shows variable nitrogen to boron ratio. We calculated

variable N:B ratio from 0.7 to 1.11 in our samples, which clearly signifies nitrogen-rich or boron-rich h-BN regions. UV-Vis spectroscopy confirms a very sharp absorption peak near 203 nm corresponding to a bandgap of 6.1 eV.

The evolution of these morphologies is attributed to the alteration of N:B ratio evolved by the mass of the AB, which has a significant impact on the decomposition process. N:B ratio can be tuned by the decomposition monitoring of ammonia borane in order to get better control over the shape of synthesized h-BN domains. Furthermore, optimal AB decomposition conditions will be investigated by the AB mass, AB heating profile, background pressure and concentration of carrier gasses to get direct access to N:B ratio.

In summary, the shape of the h-BN domains can be used as a direct indicator of nitrogen-rich or boron-rich growth. Certainly, variation in the shape of domains will influence the intrinsic and functional properties of grown h-BN layers. These results envisage that depending on the shape of individual h-BN domains, CVD synthesis will lead to either nitrogen-rich or boron-rich in-plane regions of the 2D h-BN.

References

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