CONCEPTUAL DESIGN OF INDUCTIVELY HEATED CVD REACTOR FOR HEXAGONAL BORON NITIDE SYNTHESIS

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Due to their atomically smooth surface and free dangling bonds, mono and few layer hexagonal boron nitride (h-BN) have a significant potential to be used as two-dimensional dielectric materials in functional 2D heterostructures devices [1]. Similar to graphene, controlled synthesis of large-area high-quality h-BN is important from both fundamental and applications point of views. Indeed, such applications require large scale continuous h-BN films not yet available from standard cleavage techniques. Here, we investigate the conceptual design of a new reactor built for CVD h-BN single crystals growth on copper substrates inductively heated [2]. We mainly designed a new feed system to incorporate suitable solid and liquid precursors allowing more versatility and flexibility to the process. Specifically, our design uses solid ammonia borane (AB) with independent heating control upstream of the h-BN growth, and the growth can be assisted by liquid water [3]. The choice of ammonia borane H_3BNH_3 as source material is justified by its stoichiometric quantities of boron and nitrogen, whereas water allows controlling nucleation density thereby improving h-BN grain size up to 330 µm [3]. Nevertheless, as highlighted by several reports, heating method of AB constitute the major engineering challenge towards full process control. Polymerization and foaming of AB present an additional challenge. Due to the complexity of AB decomposition, we performed a systematic thermochemical study by using *Chemkin-Pro* software to explore homogeneous gas mixture in H B N O system issued from AB precursor decomposition in argon at standard temperature of 60 °C up to h-BN growth temperature of 1140°C - beyond copper melting point. Note that at temperatures above 100 °C the ammonia borane was found to melt, coating the chamber in a white layer. In our approach, detailed model including 62 boro-nitrogen-oxygen species is performed in the specific growth condition to understand how species behaves upon vaporization from the AB precursor down to the hot regions in the vicinity of the copper substrate. Our calculation gives insight into the relative concentrations of h-BN precursor growth such as borazine ($H_3N_3B_3H_3$) as well as nucleation density regulator (HBO) Figure 1 (a-b) respectively. Elucidation of these details facilitated synthesis of high quality large area monolayer hexagonal boron nitride with safety and operational precautions considerations.

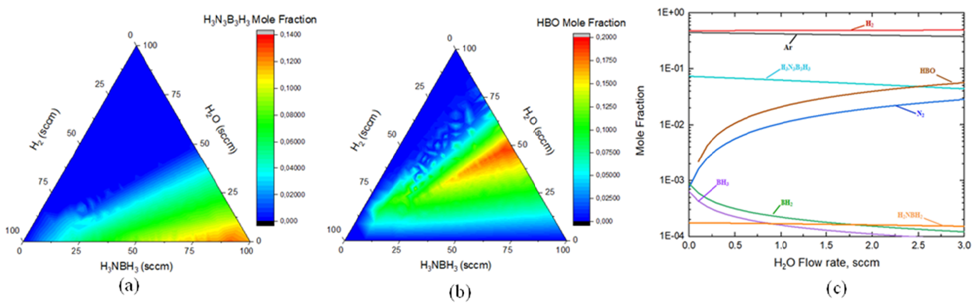

Figure 1: Ternary contour plots of (a) borazine ($H_3N_3B_3H_3$) and; (b) (HBO). Calculated at different gases flow rates at 1140°C, 1 bar and constant argon flow rate of 20 sccm. (c) Effect of water flow rate on major species distribution calculated with input flowrates H_2=1.5 sccm and AB=10 sccm.

References

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