Interplay of Kinetic Limitations and Disintegration: Selective Growth of Hexagonal Boron Nitride and Borophene Monolayers on Metal

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The CVD growth of bi-elemental 2D-materials by using molecular precursors involves complex formation kinetics. Kinetic limitations for diffusion and nucleation cause a high density of small domains and large number of grain boundaries. Naively, these are overcome by increasing the growth temperature and decreasing the growth rate. In contrast, molecular precursors exhibit limited thermal stability which can result in dissociation and preferential desorption. We demonstrate these constraints in a combined LEEM, μ-diffraction, and high-resolution LEED study by examining the selective formation of single layer *h*BN [1] and borophene [2] on Ir(111) using a borazine precursor. We derive a temperature–pressure phase diagram and apply classical nucleation theory to describe our result. We find a large critical nucleus $i^* > 8$ resulting in an almost linear dependence of island- or grain density n_{hBN} with dosing pressure p_{dose} [3]. Considering the competing processes, we find an optimum growth temperature for *h*BN of T_g = 950 °C. At lower temperatures, the *h*BN island density is increased, while at higher temperatures the precursor disintegrates and borophene is formed [3]. Studying the kinetics of borophene formation through segregation from subsurface Ir bulk regions during cool-down shows that surface steps are bunched during the borophene formation, resulting in elongated and extended borophene domains with exceptional structural order [2].

References

[1] M.A, Kriegel et al., Appl. Surf. Sci. **624** (2023) 157156
[2] K.M. Omambac et al., ACS Nano **15** (2021) 7421
[3] K.M. Omambac et al., ACS Nano **17** (2023) 17946

Figures

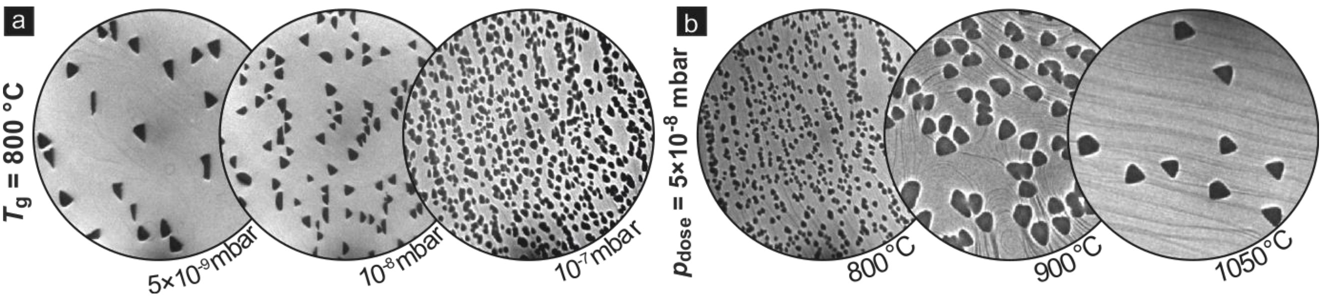

Figure 1: LEEM images showing variations in *h*BN island density n_{hBN} on Ir(111) dependent on the borazine dosing pressure p_{dose} and the growth temperature T_g. (a) An increase of n_{hBN} is observed for T_g = 800 °C while increasing p_{dose} from 5×10^{-9} to 10^{-7} mbar. (b) A decrease of island density *nh*BN is observed for p_{dose} = 5 × 10^{-8} mbar while increasing T_g from 800 to 1050 °C.