

# Competing Processes as a Quality Limitation: New Insights into Microscopic Growth Mechanisms of Single-Layer Hexagonal Boron Nitride on Ir(111)

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The structural quality of 2D materials (2DMs) critically affects their properties: while fewer defects improve electron mobility [1] and excitonic behaviour [2], engineered defects enable single-photon emission [3]. Yet, microscopic insights into quality-determining mechanisms remain limited. Here, we investigate the structural quality of single-layer hBN grown epitaxially on Ir(111), focusing on a variety of structural defects, including grain boundaries, wrinkles, and rotational domains. The Island density, determined via high-resolution low-energy electron diffraction and low-energy electron microscopy as a function of substrate temperature  $T_g$  and dosing pressure ( $p_{\text{dose}}$ ), reveals two key processes (Fig. 1a): (i) borophene formation under conditions where borazine decomposes (orange area, panel b) [4], and (ii) a strong  $p_{\text{dose}}$  dependence, that increases the density of grain boundaries (panel c). Together, these effects set a fundamental quality limit for CVD-grown hBN and other 2DMs [5].

## References

- [1] L. Cheng, Y. Liu, *J. Am. Chem. Soc.* **140** (2018) 17895
- [2] A. Sharma, M. Hasan, Y. Lu, *Mater. Futures* **1** (2022) 042001
- [3] N. Mendelson et al., *ACS Nano* **13** (2019) 3132
- [4] K. Omambac et al., *ACS Nano* **15** (2021) 7421
- [5] K. Omambac et al., *ACS Nano* **17** (2023) 17597

## Figures

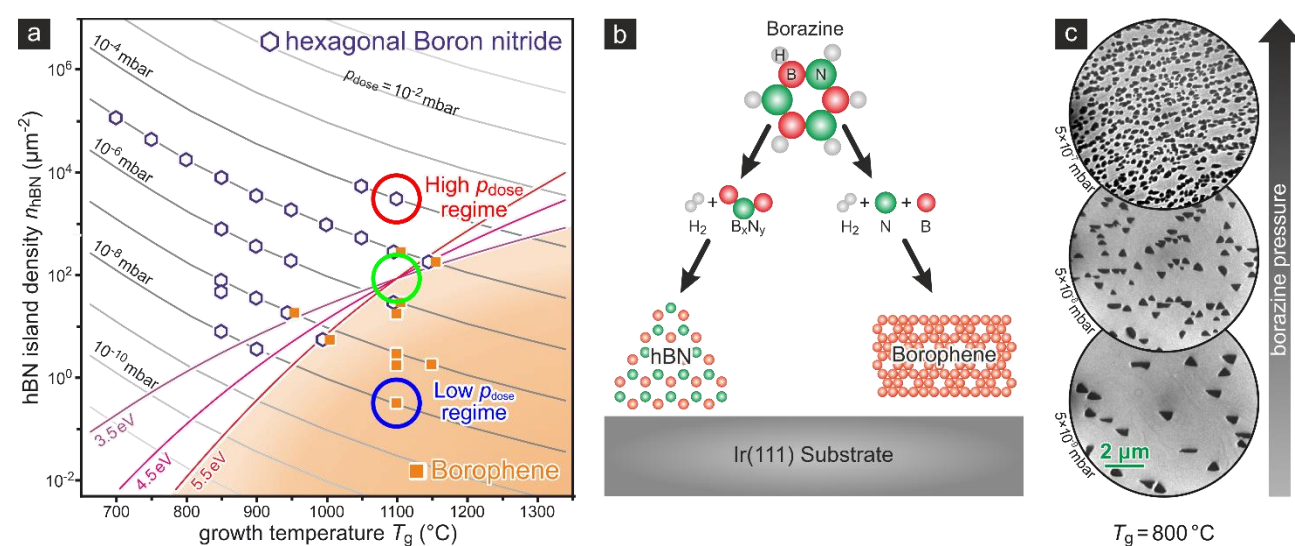


Figure 1: Processes during growth of hBN on Ir(111). The phase diagram (a) clearly reveals two key features of the material system during low-pressure CVD growth: The growth of borophene and hBN from a single precursor (b) and the formation of grain boundaries with increasing dosing pressure (c).