Hexagonal boron nitride crystal growth from iron, a single component flux

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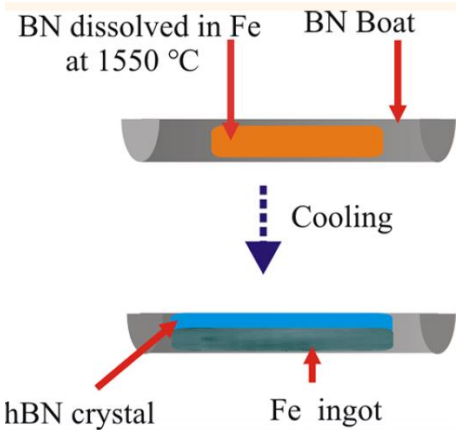
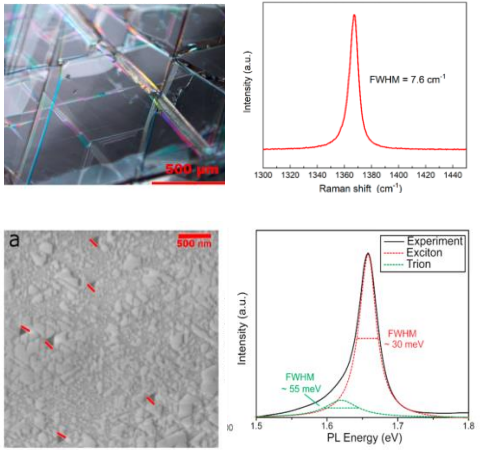
Project Summary: The highest quality hexagonal boron nitride (hBN) crystals are grown from molten solutions. For hBN crystal growth at atmospheric pressure, typically the solvent is a combination of two metals, one with high boron solubility and the other to promote nitrogen solubility. This study demonstrates that high quality hBN crystals can be grown at ambient pressure using pure iron as a flux which is unexpected given the low solubility of nitrogen in iron. The properties of hBN crystals produced using an iron flux match the best values ever reported for hBN: a narrow Raman E_{2g} vibration peak (full-width-at-half-maximum=7.6 cm^{-1}) and strong phonon-assisted peaks in the photoluminescence spectra. To further test their quality, the hBN crystals were used as substrates for WSe_2 density which revealed a low nucleation density indicating a low defect density in the hBN. The ability to produce high quality hBN crystals in a simple, environmentally friendly and economical process will advance 2D materials research by enabling integrated devices. Published in: *ACS Nano* 2021, 15, 7032-7039.

2DCC Role: The use of WSe_2 epitaxy as a diagnostic technique to evaluate point defect levels in hBN is based on theoretical and experimental results previously published by the 2DCC in-house team (See *ACS Nano* 2019, 13, 3341-3352). Epitaxial growth of WSe_2 was carried out by metalorganic chemical vapor deposition in the 2DCC facility on hBN crystals supplied by the external user.



Schematic illustration of hBN crystal growth using the single component Fe flux method.



(Top row) Transparent hBN crystal and Raman spectrum showing narrow E_{2g} peak. (Bottom row) Low density of WSe2 nuclei (marked in red) on hBN surface and corresponding photoluminescence spectrum.