

SINGLE CRYSTAL MONOLAYER GRAPHENE AND HEXAGONAL BORON NITRIDE BY INDUCTIVE HEATING CVD

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The reduced dimensionality of 2D materials induces all surface accessible defects which play a critical role in materials' properties and device performance. One common defect in 2D materials is the grain boundaries (GBs) consisting of a series of pentagon, heptagon, and hexagon rings formed at the stitching region between two domains with different orientations (Fig 1a). To control the orientation of these domains, monocrystalline Cu(111) is used for graphene growth due to the absence of GB and the small mismatch (Fig 1b). In our approach, centimeter-scale single crystal Cu(111) is produced by applying a controlled thermal gradient to a commercial polycrystalline copper substrate using inductive heating. A 25 μm thick copper foil was transformed into a single-crystal copper foil by inductively heating to $\sim 1030^\circ\text{C}$. Unlike Roll to Roll (R2R) methods where the copper is continuously passed in a hot furnace region [1], in our approach, the induction coils are moved at the speed of 1 cm/min (Fig 1c). An edge of the Cu sheet was tapered into a tip shape, which ensured the nucleation of a single Cu(111) grain at the tip. The sliding of the coils across the copper foil caused the movement of the grain boundaries between the single crystal and polycrystalline regions and the grain of single crystal Cu(111) reached the width of the copper sheet. X-ray diffraction of the copper obtained showed the presence of the (111) preferential direction (Fig 1d). 3D calculation demonstrated the driving force of the thermal gradient for the Cu(111) formation (Fig 1e). Consequently, graphene and hexagonal borane nitride were synthesized using inductive heating. From the optical microscopy image (Fig 1f), we can see that all the hexagonal graphene domains are oriented in the same direction and the Raman spectrum shows the total absence of defects (inset f). By applying the same concept to CVD h-BN growth on Cu(111) from ammonia borane, triangular and oriented domains of hexagonal boron nitride are obtained (Fig 1g). During the growth, the adjacent flakes coalesce or compete for adatoms during the growth following the point-to-edge model [2].

References

- [1] X. Xu et al., Science Bulletin 2017, 62(15) pp.1074-1080.
- [2] Liu et al, Nano Materials Science, 3, (2021) pp 291-312

Figures

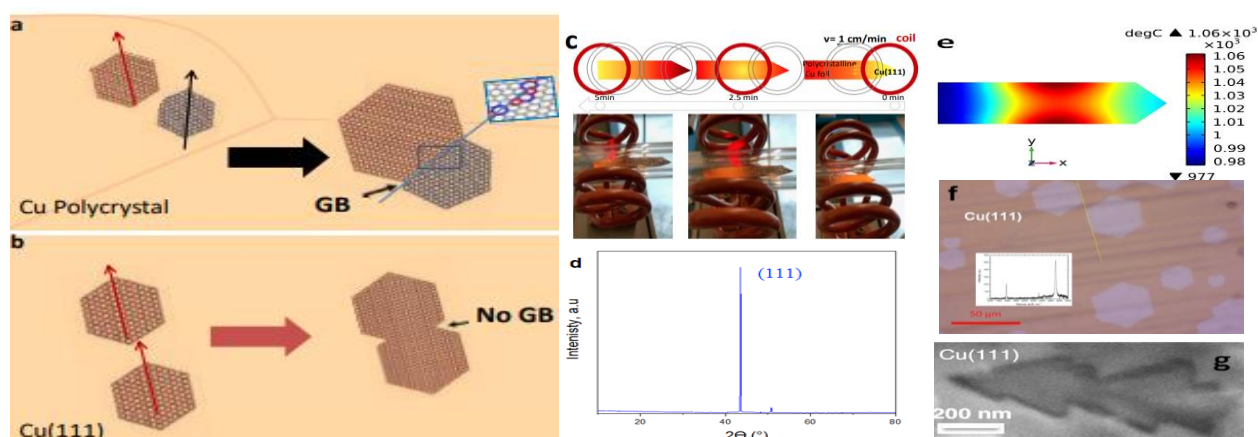


Figure 1: **a,b** Effect of Cu crystallinity on Gr grain boundaries (GB); **c** Inductive heating synthesis of Cu(111); **d** XRD spectra of Cu(111); **e** Comsol 3D calculation of thermal gradient for Cu(111); **f** Optical image of oriented graphene domains on Cu(111); Inset **f** Graphene Raman spectra obtained with 473 nm laser excitation on copper foil; **g** Oriented triangular hBN domains.