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Understanding and improving the properties of polycrystalline graphene: Synthesis and Simulations

Graphene's mechanical properties are superior due to its low dimensionality and defect density. The immense strength of graphene was first measured through the nanoindentation of suspended circular membranes; proving graphene to be the strongest material ever characterized [1]. In an effort toward scalable and reliable production, chemical vapor deposition (CVD) methods on copper substrates have proven to be a fruitful method to synthesize large-area monolayer polycrystalline sheets of graphene. While grain boundaries are consequently introduced during synthesis, subsequent nanoindentation methods have shown the strength is still significant. Herein we present methods to significantly improve the quality of CVD-grown graphene. First, we employ rotating-disk electropolishing of copper substrates to obtain nanometer-scale surface roughness over large areas. This allows for control over nucleation density and leads to improved transfer methodologies. Second, the construction of an ultra-high-purity, custom-designed CVD furnace utilizes high-quality purifiers to reduce the oxygen contamination to one part per-billion. This significant reduction in oxidizing species significantly improves growth rate and domain size [3]. Lastly, we further optimized existing electrochemical delamination techniques of graphene from the ultra-flat copper substrates. The combination of these factors is expected to lead to improved and more consistent material properties of CVD-grown graphene; in particular, better-stitched grain boundaries. In parallel, we have formulated a semi-analytical probability density function (PDF) of the critical failure load for polycrystalline two-dimensional materials that we seek to validate against future nanoindentation experiments in order to more accurately understand the mechanical properties of grain boundaries in graphene.

References

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