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The mechanical properties of grain boundaries in chemical vapor deposition grown graphene: Simulations and Experiments

Graphene is the strongest material ever characterized. Its elastic modulus and mechanical strength were first measured through the nanoindentation of free-standing circular membranes [1]. In order to take advantage of graphene's strength in an industrially scalable manner, chemical vapor deposition methods have been developed to synthesize large area continuous monolayer films. Although the subsequent films contain grain boundaries, nanoindentation experiments demonstrate they still achieve a significant portion of their fracture [2]. Herein, we utilize oxygen assisted methods to allow tunability in the nucleation density. We present electropolishing techniques of copper to consistently achieve nanometer scale surface roughness over large areas. This yields an increase in nucleation uniformity, as well as a more mechanically robust film. These methods allow for more meaningful statistics to be built from experiments. In parallel, we present a numerical formulation for a membrane-based cohesive zone model to model the fracture of grain boundaries in graphene through the finite element method within the context of the nanoindentation experiment. Our failure analysis provides a relationship between the critical failure load and the distance of the grain boundary. The results are used to calculate a probability density function of polycrystalline graphene that can be validated against the nanoindentation experiments to understand the mechanics of failure of grain boundaries in graphene.

References

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[2] Gwan-Hyoung Lee, Ryan C. Cooper, Sung Joo An, Sunwoo Lee, Arend van der Zande, Nicholas Petrone, Alexandra G. Hammerberg, Changgu Lee, Bryan Crawford, Warren Oliver, Jeffrey W. Kysar, and James Hone, Science, 6136 (2013) 1073–1076

Figures

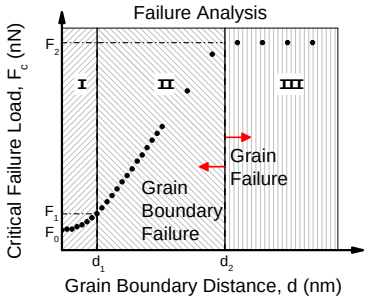

Figure 1: Relationship between the critical failure load and the grain boundary distance in a nanoindentation experiment.