A multiscale model of the failure of polycrystalline CVD-grown graphene subject to nanoindentation

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Abstract

Single crystal graphene has been proven to be the strongest material ever characterized through the nanoindentation of free-standing circular membranes [1]. While chemical vapor deposition offers an industrially scalable path to generate large area sheets of graphene, it introduces defects into the lattice in the form of grain boundaries. Nanoindentation experiments of the resulting polycrystalline film demonstrates a slight reduction in strength that can be attributed to the grain boundaries [2]. In order to understand the mechanical behavior of these grain boundaries and the probability of failure, we present a multiscale model of the nanoindentation of polycrystalline graphene through the finite element method. We have developed a membrane-based cohesive zone model (CZM) to simulate the grain boundary rupture. To validate the CZM, we examine the transition in failure mechanisms from one of elastic instability to one of grain boundary rupture based on the proximity of the grain boundary to the indenter tip and variation of the indenter tip radius. We finally examine the probability of failure with both a periodic and a random grain structure and compare the results with nanoindentation experiments.

References

[1] Changgu Lee, Xiaoding Wei, Jeffrey W. Kysar, and James Hone, Science, 5887 (2008) 385-388
[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

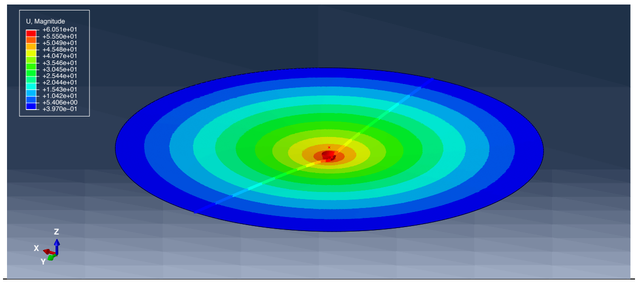

Figure 1: Perspective view of the displacement magnitude of the nanoindentation of a free-standing circular membrane with a single straight grain boundary running directly through the center at failure

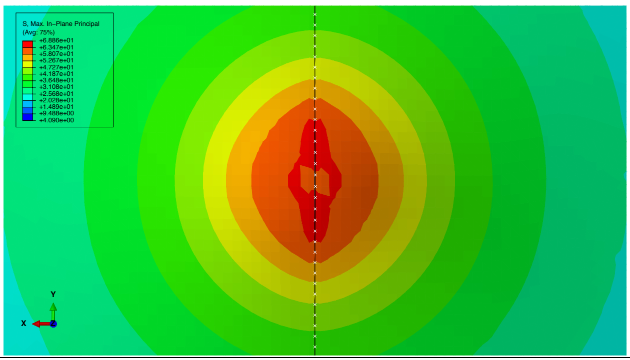

Figure 2: Maximum In-plane Cauchy stress at the point of failure immediately beneath the indenter tip with a single straight grain boundary running directly through the center