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Can We Map the Fracture Force from Nanoindentation into the Strength of Graphene under Tensile Loading?

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ABSTRACT

Due to the difficulty of performing uniaxial tensile testing, the strengths of graphene and its grain boundaries have been measured in experiments by nanoindentation testing. From a series of molecular dynamics simulations, we find that the strength measured in uniaxial simulation and the strength estimated from the nanoindentation fracture force can differ significantly. Fracture in tensile loading occurs simultaneously with the onset of crack nucleation near 5-7 defects, while the graphene sheets often sustain the indentation loads after the crack initiation because the sharply concentrated stress near the tip does not give rise to enough driving force for further crack propagation. Due to the concentrated stress, strength estimation is sensitive to the indenter tip position along grain boundaries. Also, it approaches the strength of pristine graphene if the tip is located slightly away from the grain boundary line. Our finding reveal the limitations of nanoindentation testing in quantifying the strength of graphene, and show that the loading-mode-specific failure mechanism must be taken into account in designing reliable devices from graphene and other technologically important 2D materials.

1. INTRODUCTION

Polycrystalline graphene synthesized by chemical vapor deposition is an inevitable choice for the realization of graphene device requiring large-area graphene. To understand the effect of grain boundaries (GBs) on the strength, nanoindentation testing has been performed due to the difficulty of performing uniaxial testing. However, the outcomes from several experiments are not consistent with each other; some reported the GB strength is comparable to the pristine one (Lee 2013), while the others reported that the former is significantly weaker than the other (Rasool 2013). Meanwhile, in atomistic uniaxial tensile simulations predict that the strength of GB is lower than the pristine graphene due to the pre-stress build up around 5-7 defects along GBs (Wei 2012). In this study, we perform molecular dynamics simulations to

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compare the predicted strength as well as the failure mechanism in both uniaxial tensile simulations and nanoindentation simulations.

2. The Cause of the Inconsistency Among Nanoindentation Experiments.

We find two cause of the inconsistency among nanoindentation experiments. First, in nanoindentation, failure of graphene does not immediately follow the crack nucleation, while it does in uniaxial tensile tests. (Fig. 1a) Second, the failure force in nanoindentation is very sensitive to the distance between the GB and the indentor tip. Thus, a slight misalignment may lead to significantly different results. (Fig. 1b)

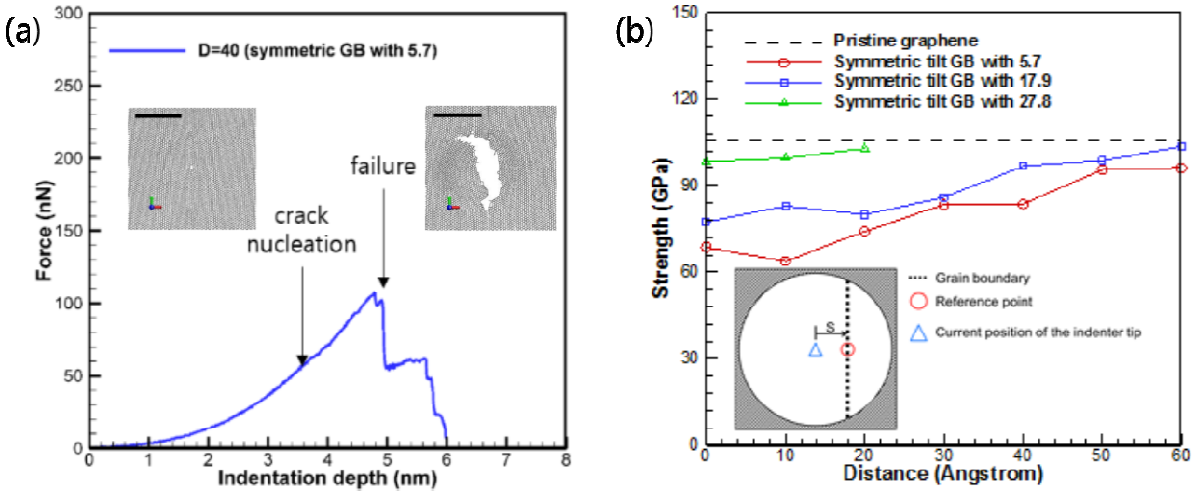

Fig. 1 (a) Failure mechanism of GB under nanoindentation (b) Strength measured as a function of the distance between the GB and indentor tip

We find that such a delayed failure after crack nucleation occurs only for the small tilt angle GBs, and overestimate its strength. Thus, the GB strength is likely to be overestimated in nanoindentation. Also, a slight misalignment (about the radius of indentor tip) leads to the strength estimation comparable to the pristine graphene. Considering very small indenter tip size (~100nm) in experiments, the GB strength may have been overestimated due to the indenter misalignment.

3. CONCLUSIONS

Our finding reveal the limitations of nanoindentation testing in quantifying the strength of graphene, and show that the loading-mode-specific failure mechanism must be taken into account in designing reliable devices.(Han 2015)

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