

Adhesion of Graphene Sheets

with Crystallographic Registry and Misorientation



Northeastern University Research & Scholarship Expo 2009

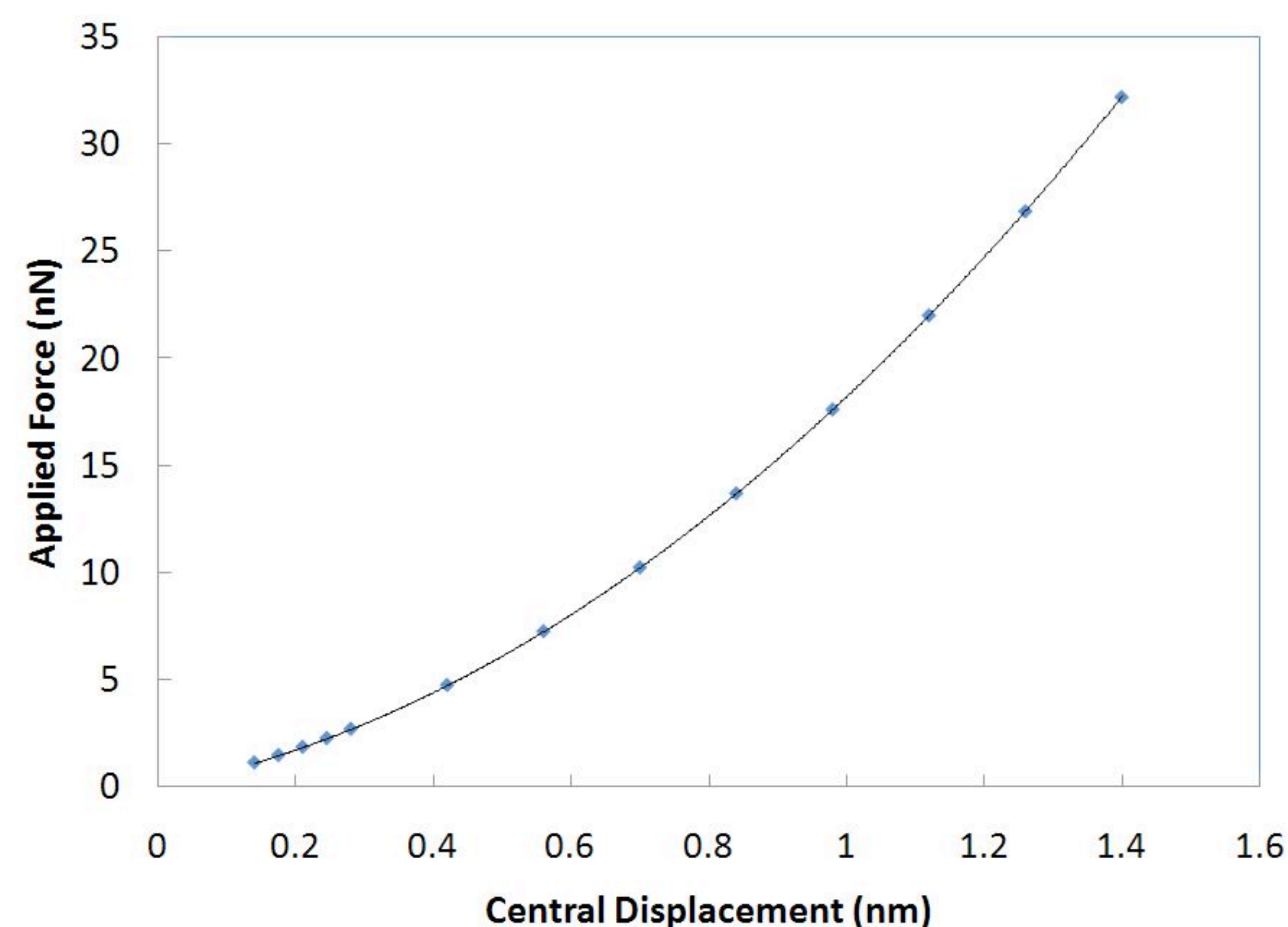
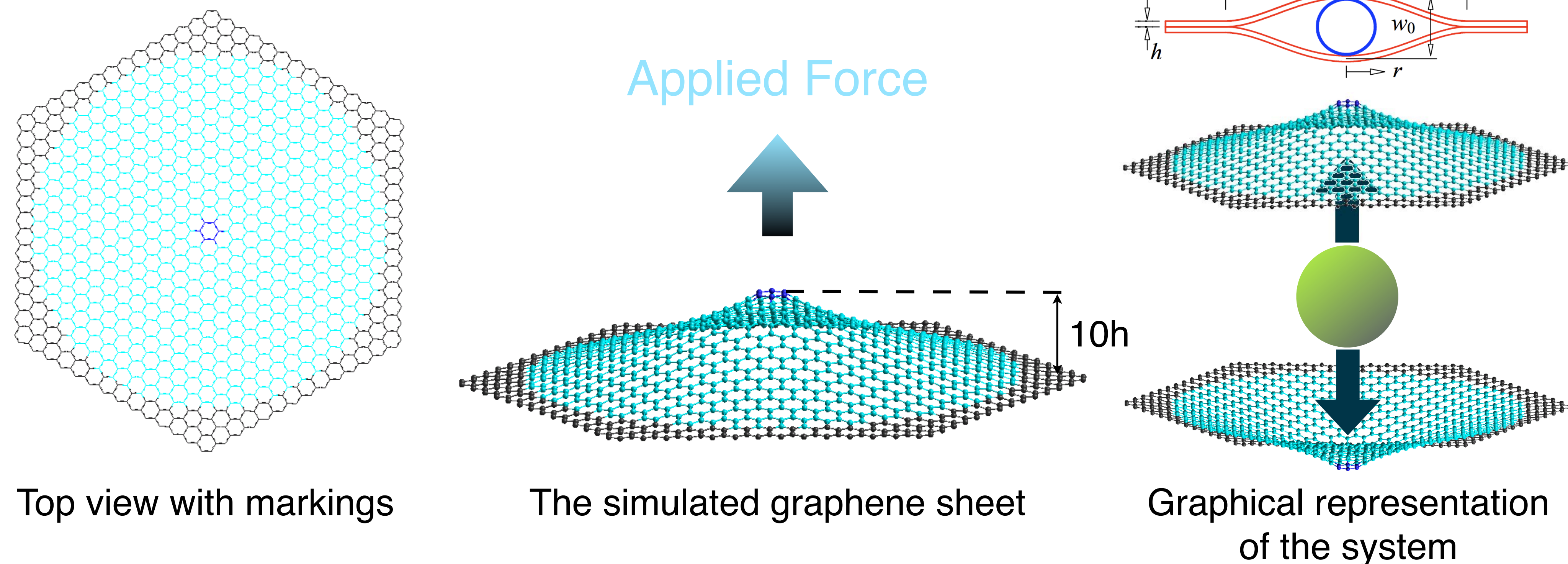
Yung Kong Fan and Kai-Tak Wan
Mechanical & Industrial Engineering, Northeastern University, Boston, MA

1. Introduction

Graphene sheet, being the building block of graphite, comprises layers of carbon arranged in a hexagonal pattern. The nano-structure is crucial in the latest development of nano-science and nano-technology with applications ranging from composite materials, drug delivery, flexible electronics and circuitry, micro-/nano-electromechanical systems (MEMS / NEMS) etc. A comprehensive understanding of graphene in terms of optical, electrical, mechanical, chemical behavior is therefore necessary. This research focuses on the mechanical aspects.

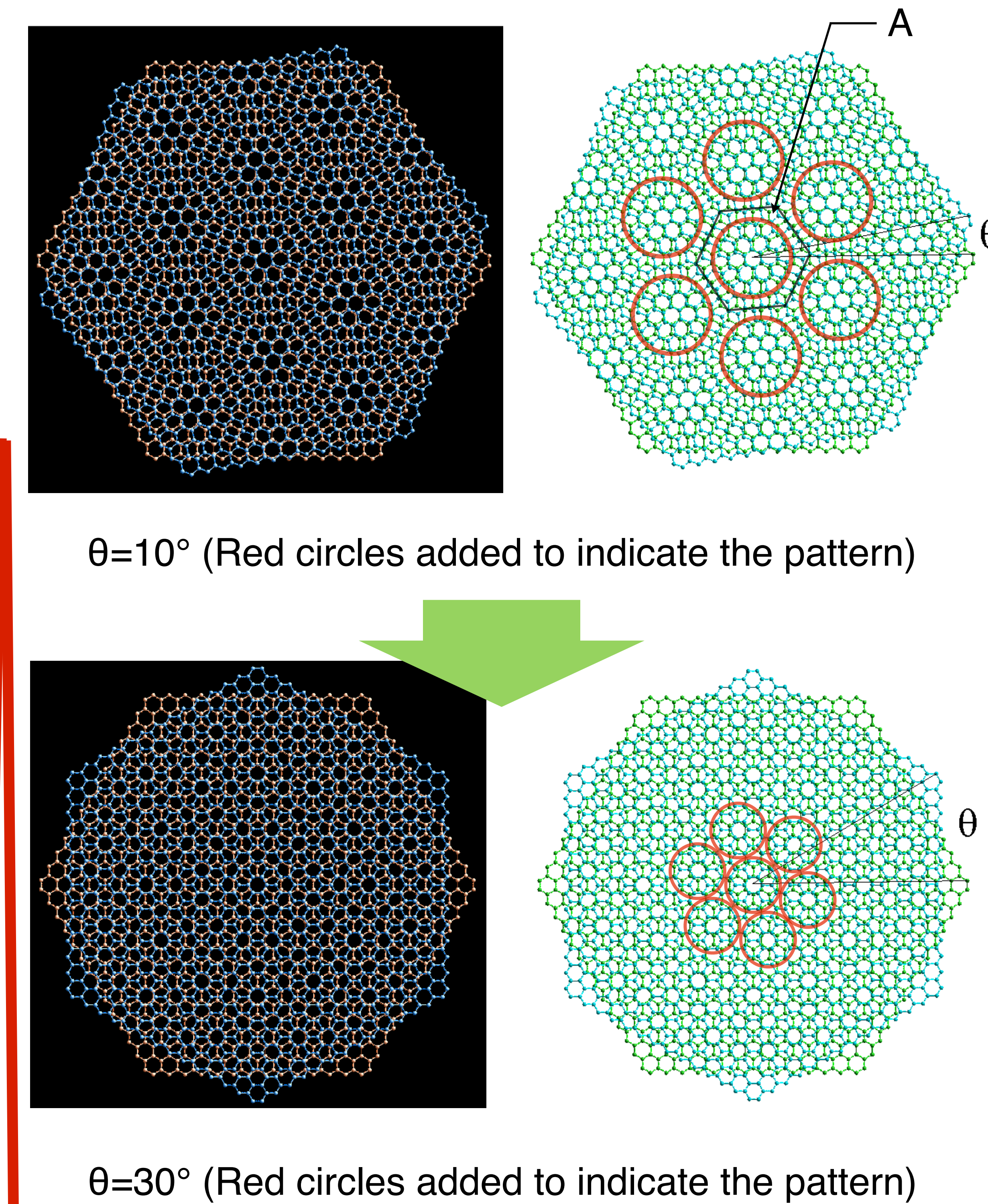
Upon loading by an external load, the graphene sheet deforms according to its linear elastic constitutive relation. Should the external force be replaced by an intrinsic intersurface interaction, the sheets adhere and form multi-layered structure. We investigate the coupled mechanical deformation and adhesion-delamination using Molecular Dynamics Simulation (MDS) based on Molecular Mechanics (MM+). Adhesion between sheets with crystallographic registry and misorientation are studied.

2. Mechanical Deformation

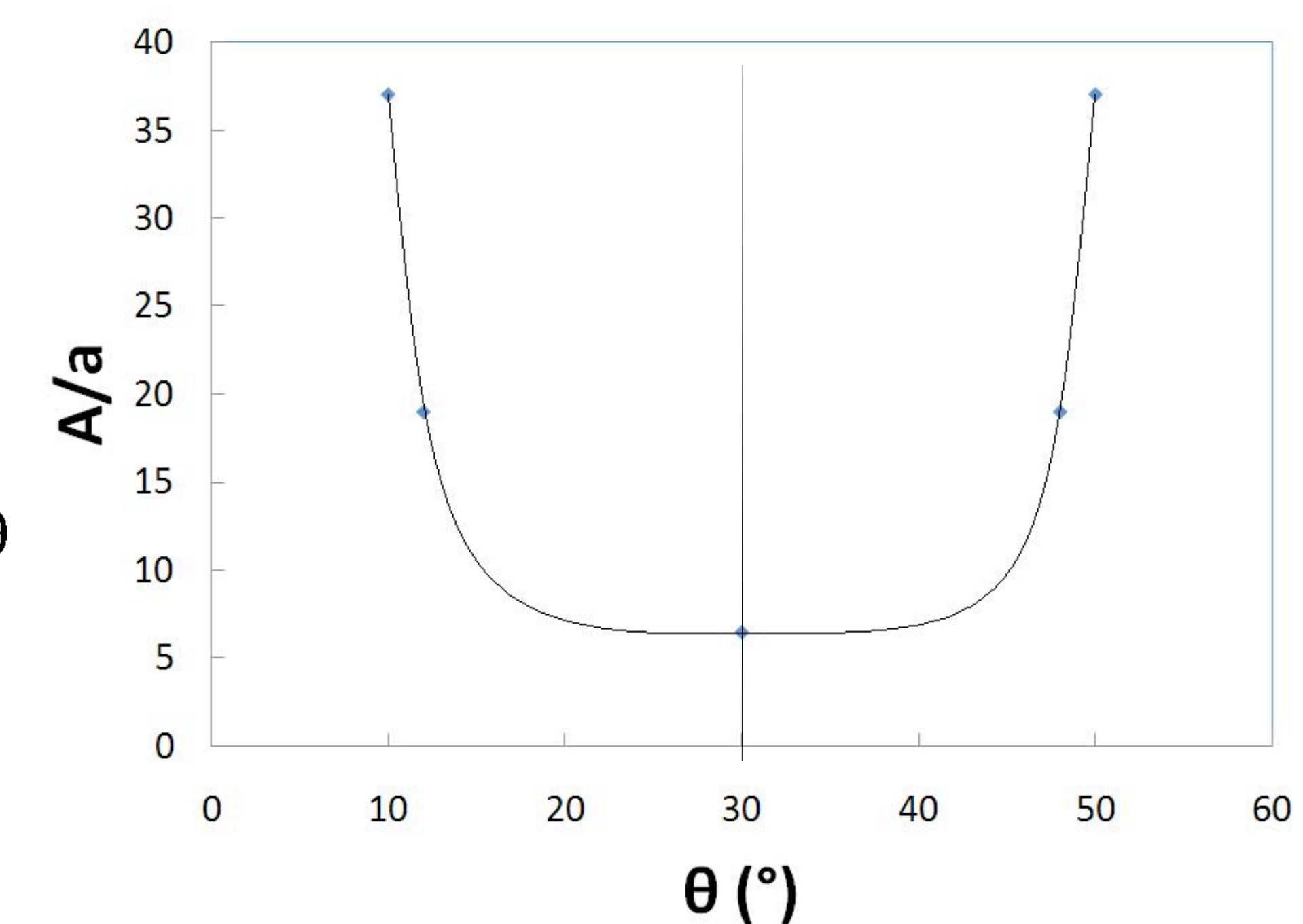


The graphene sheet is represented by a ball-stick model. The dark atoms are fixed in position denoting an adhered interface, while the blue are free to deform denoting the "crack" area. The central 6-member ring is raised by $10h$ resulting in the "cusp" geometry. The central load can be applied externally, yielding a force-displacement curve as shown. A bilayer structure can be wedged by a particle trapped at the interface. A large particle causes the circular contact edge to expand, indicating the interfacial adhesion energy.

3. Crystallographic Registry



When two identical graphene sheets adhere with a non-zero mis-orientation angle θ , a Moire interference pattern is generated. Area of the super hexagons follows a sinusoidal variation with a period of $\theta = 60^\circ$ period conforming to the hexagonal symmetry. Minimum is reached at a multiple of 30° .



Area of hexagonal ring formed by linking the midpoints between the central pattern's center and the repeating patterns' (A) over area of unit carbon ring (a) vs. Misorientation angle (θ)

4. Conclusion

Materials parameters (e.g. elastic modulus and area extensional modulus) will be extracted from the force-displacement curve obtained for a range of blister dimension. These numbers are expected to vary from macro- to nano-scale, because the crystallographic nature prevails as the sample dimension shrinks below a certain threshold. Comparison between theoretical computation and experimental data will be carried out. Experimental verification will be conducted for graphene adhesion. Large graphene sheets are peeled from graphite block, while nano-particles serve as central wedges.

Molecular dynamics simulation is used to deduce the mechanical and adhesion behavior of graphene sheets. Graphs and trends provide first order approximation for empirical investigation in the future. Such computation and experiments are essential to probe the mechanical behavior of nano-structures in general.

Support from Provost's Office Undergraduate Research Grant and National Science Foundation (NSF-CMMI-0757140) is acknowledged. We are grateful to Dr. Zong Zong also for helpful discussion.

Future work

Conclusion of this research

Acknowledgement