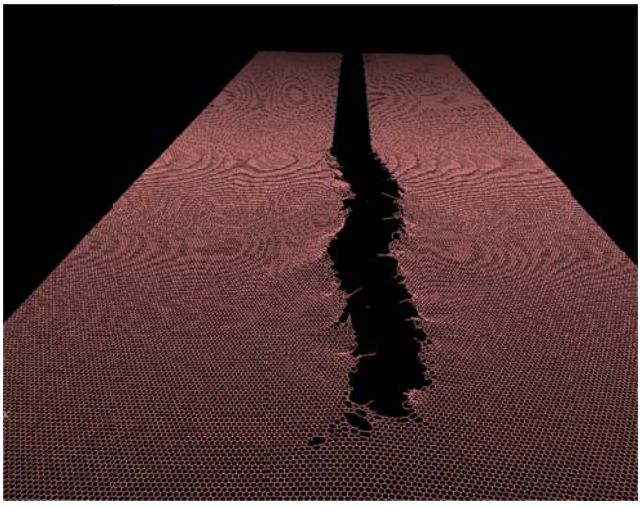
Project Title: Mechanisms of nano-scale grain boundary toughening in Graphene

Advisor: Prof. H.B. Chew

Project Description:

Graphene, the one-atom-thick sheet of carbon, is the strongest and thinnest material in the world, and holds considerable promise in a wide array of engineering devices and applications. Recent state-of-the-art manufacturing methods have led to the production of macroscopic-scale graphene films, which represents an important step for massive scaling-up of graphene technology. A major obstacle, however, is that the as-produced graphene film is highly polycrystalline with unknown mechanical properties. An important step will be to develop methods to assess the fracture characteristics of the individual graphene grain boundaries. In this research, you will be studying the fracture response and toughness of graphene grain boundaries using molecular dynamics solver LAMMPS. You will also be gaining experience on how well-established continuum fracture theories, like the *J*-integral, can be used to measure atomic-scale toughness in the simulations.



Student background and expected research activities:

We are looking for an enthusiastic and motivated individual, with a sense of curiosity about the atomic world. No prior experience or previous knowledge of molecular dynamics is needed.

Points of contact:

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