Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Effective structural properties in polycrystalline graphene ZUBAER HOSSAIN, University of Delaware — This talk will discuss effective structural properties in polycrystalline graphene under the presence of atomic scale heterogeneity. Polycrystallinity is ubiquitous in solids, but theories describing their effective behavior remain limited, particularly when heterogeneity is present in the form of nonuniform deformation or composition. Over the decades, exploration of the effective transport and strength properties of heterogeneous systems has been carried out mostly with random distribution of grains or regular periodic structures under various approximations, in translating the underlying physics into a single representative volume element. Although heterogeneity can play a critical role in modulating the basic behavior of low-dimensional materials, it is difficult to capture the local characteristics accurately by these approximations. Taking polycrystalline graphene as an example material, we study the effective structural properties (such as Young's Modulus, Poisson's ratio and Toughness) by using a combination of density functional theory and molecular dynamic simulations. We identify the key mechanisms that govern their effective behavior and exploit the understanding to engineer the behavior by doping with a carefully selected choice of chemical elements.

Zubaer Hossain
University of Delaware

Date submitted: 21 Oct 2015 Electronic form version 1.4