

NANOMECHANICS OF GRAPHENES AND NANOCRYSTALS

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Nanomechanics understandings for nanostructures are critical not only for their integrity concerns but also for their utilization. Attention here is focused on two types of low-dimensional materials, graphenes and nanocrystals, with characteristic lengths in nanometers or even angstrom scales. In nanocrystals, the dislocation mechanism is suppressed, and their plasticity is dictated by diffusive atomistic flow along the grain boundaries. Micromechanics models are developed for the plastic flow and fracture in nanocrystals. Simulations based on micro-structural evolution demonstrate the capability in predicting the brittle versus ductile transition of nanocrystal. To put this mechanism into atomistic images, in-situ tests of nanocrystalline gold were performed under HRTEM. We observe atoms flow along certain atomistic planes of the crack faces to advance the crack. This diffusion assisted mode, along with GB cavitation and cleavage, give a complete spectrum of defect evolutions in nanocrystals.

Beside the danger of to degrade the nanostructures, defects may also serve to enrich the functions of nanostructures. The functioning of pristine graphenes is rather difficult. Doping of graphenes, however, can be achieved along their edges. We collaborated with a group in KAUST to study the defect creation and evolution in graphenes. The HRTEM there can operate at low voltage but with 1.1 angstrom resolution. We devise a two-step method for atomic doping of graphene: the first step consists of creating holes and vacancies in graphene by bombardment of Au atoms, while the second step consists of doping atoms of various kinds to the edges of the hole and into the atomic vacancies. These doping atoms serve to functionalize the edges and to create catalysts in the form of single atom arrays. The mechanics of graphene is also explored by observing the atom-resolved mode-III fracture process in graphenes, and by elucidating the failure mechanisms of graphene nano-ribbon.

Keywords: Nanomechanics; graphene; nanocrystal;