Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Mechanical properties and interface of carbon/metal nanocomposites

Cranford, Steven, s.cranford@neu.edu; Roman, Ruth, Northeastern University, United States

ABSTRACT

The recent discovery of graphene and its associated thermal, electrical, and mechanical properties has motivated further investigation of similar two-dimensional (2D) systems, including all-carbon allotropes of graphene. The high strength and atomistic thickness of such 2D systems make them promising for composite materials. However, there is intrinsic weakness at the interface, typically characterized by noncovalent interactions. Here, we present two nanocomposite studies: mechanical properties of graphdiyne/copper composites and defect engineering of graphene/copper interfaces.One emerging allotrope of graphene is so-called graphdiyne, a one atom-thick carbon network which can be constructed by connecting two adjacent hexagonal rings with uniformly distributed diacetylenic linkages. This allotrope has demonstrated a set of distinguished properties and is considered a promising material, which can meet the increasing requirements to carbon-based nanomaterials. There are a few reports of the mechanical behavior of isolated graphdiyne. However, currently graphdiyne has only successfully been synthesized on copper substrates, and the composite behavior of the material has not been investigated. Here, we combine copper/graphdiyne nanocomposites with varied numbers of layers of graphdiyne sheets, as well as sandwich-structured copper/graphdiyne layers to determine mechanical properties. Using full atomistic molecular dynamics, the elastic stiffness and limit states of these nanocomposite materials are investigated through direct tensile loads. We present theoretical methods to estimate the parameters to mechanically characterize copper/graphdiyne nanocomposites. Second, we present a simple model of graphene/copper, subject to shear stress transfer across the carbon/metal interface. The weak van der Waals interaction governs the strength of the system. To increase the strength of the interface, vacancy defects are introduced into the graphene, to “rough up” the potential landscape and facilitate stress transfer. Although the strength of the graphene is decreased, the stiffness is only marginally affected, and the response of the composite system can be improved. Such defect engineering can potentially be used to enhance the compatibility of carbon/metal nanostructures.