Announcement of a virtual special issue on computational carbon nanoscience

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Editorial

Announcement of a virtual special issue on computational carbon nanoscience

The *Carbon* journal is pleased to introduce a themed collection of recent articles in the area of computational carbon nanoscience. This virtual special issue was assembled from previously published *Carbon* articles by Guest Editors Quan Wang and Behrouz Arash, and can be accessed as a set in the special issue section of the journal website homepage: www.journals.elsevier.com/carbon. The article below by our guest editors serves as an introduction to this virtual special issue, and also a commentary on the growing role of computation as a tool to understand the synthesis and properties of carbon nanoforms and their behavior in composite materials.

Since their discoveries, carbon nanotubes and graphene-based materials have been the subject of extensive investigations motivated by their extremely high strength and exceptional electronic and thermal properties. Investigations into their material properties as either single components in nanoscale devices such as nano-sensors, or as fillers in high-performance nanocomposites have become one of the most active research directions in physics, chemistry and nanotechnology. Recent findings illustrate their broad potential as enabling components in biomedicine, composites, energy storage, sensors, and other areas.

It has been broadly recognized that molecular simulation studies provide an indispensable tool for the development of nanotube and graphene-based composite materials. Simulations can provide detailed information at the molecular and atomic scales on issues such as stress–strain behavior and interfacial interactions between matrix and nano-reinforcements, and hence offer new interpretations of experimental results and guide the design of new laboratory experiments. However, molecular simulations are only efficient for systems with a limited number of atoms due to computational limits and high computational costs. In view of these limitations, continuum mechanics approaches with relatively simple formulations continue to be used in the modern carbon materials research. However, continuum models, which have been developed under basic assumptions of continuous media, are unable to adequately capture the atomic structures of nano-materials, and hence cannot efficiently achieve in-depth insights into the underlying mechanisms of phenomena at the atomic level. A verification of results obtained by continuum theories with those of molecular simulations or experiments is indispensable when applying the theories in the analysis of nano-materials. In view of the pros and cons of the above two methods, multi-scale methods have been proposed and developed for the analysis of carbon nanotubes and graphene materials, which can involve continuum and atomistic descriptions of a material at each scale. The fundamental principle of multi-scale modeling is to couple two models across multiple scales, i.e., an atomistic model to describe molecular interactions and a continuum mechanics model to simulate a set of atoms in a mesh undergoing a homogeneous deformation.

This virtual special issue is dedicated to recent developments in modeling of carbon nanotubes, graphene-based materials and their composites using molecular simulations, continuum mechanics, and multi-scale methods for predictions of mechanical and thermal properties. A wide range of fundamentally theoretical and computational topics on modeling and applications of carbon nanotubes and graphene materials can be seen by reading through the contributing papers in this issue. In addition, the set of papers serve to show the potential for carbon nanofillers in substantially enhancing mechanical and thermal properties of resulting composites. We were impressed by the number and quality of computational studies in the recent volumes of the Carbon journal. In this issue, Shariat et al. [1] used molecular dynamics simulations to show how plasma-based deposition allows low-temperature growth of nanotubes. The simulation results demonstrate how ion bombardment during the growth influences the carbon dissolution. The study extends our knowledge about the detailed mechanism of CNT growth. Cerqueira et al. [2] investigated mechanical behaviors of carbon nanotubes subjected to hydrostatic pressure using the density-functional based the tight-binding method. In view of scattered and even contradictory simulation results presented by classical molecular simulations in literature, the quantum–mechanical description provides accurate simulation results for collapse of carbon nanotubes under

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hydrostatic pressure for nanotubes with a variety of diameters and chiralities.

Han et al. [3] investigated the ultimate strength and failure mechanism of grain boundaries in graphenes with molecular dynamics simulations. The overall strength enhancement and weakening behaviors of pentagon–heptagon defects along the grain boundaries are particularly discussed. Molecular simulations were used by Gu at al. [4] in studying the effects of cone angle on mechanical properties and the failure mechanisms in carbon nanofibers made of multilayered carbon nanotubes and platelet-like graphitic fibers. The study provides a further understanding of the origin of strength dispersions observed in experiments. Ruiz et al. [5] proposed a coarse-grained molecular dynamics model of graphene, which is able to quantitatively reproduce its mechanical responses in the elastic and fracture regimes. The hierarchical multi-scale approach is expected to become a powerful method to predict the meso-scale behavior of nano-materials in the future. Thermal properties of graphene materials were explored by Liu et al. [6]. The research investigates an interface thermal conductance and interface thermal rectification of hybrid graphene/silicene monolayers by molecular dynamic simulations. The authors conducted a detailed phonon spectra analysis to examine the effects of the system size and temperature, external strain and heat flux on the interface thermal conductance of hybrid graphene/silicene monolayers. The investigations enable to take advantages of hybrid heterostructures in advanced nanodevices.

O'Brien et al. [7], and Filleter and Espinosa [8] introduced a novel method to improve mechanical properties of single-walled carbon nanotube bundles through carbon ion irradiation using molecular dynamics and multi-scale approach. The simulation results demonstrate that carbon-ion irradiation not only induces nanotube cross-links, but also causes defects. The cross-links are formed in different types from simple direct bonds between nanotubes to complex links between interstitial compounds. Dispersion of carbon nanotube bundles in different solutions by applying torsional energy was investigated by Wu et al. [9] using molecular dynamics simulations. From the simulations, the torsional energy applied on the two ends of the bundles results in a local buckling of the structures. The impulse between carbon nanotubes due to the local buckling generates the driving force through a process of releasing the energy. This paper provides an effective method for dispersion of carbon nanotubes from their bundle structure. Molecular dynamics simulations were used to evaluate the effect of the volume fraction of nanotube reinforcements on mechanical properties of multi-walled carbon nanotube/polyimide composites [10]. The simulation results provide insights on how the polymer chains may interact with long nanotubes.

Yang et al. [11] used molecular simulations to investigate the effect of the Thrower–Stone–Wales defect on the elastic stiffness of carbon nanotube/polypropylene composites and the adhesion characteristics of polymer crystallization on the surface of nanotubes. The authors have reported the improvement of the interfacial adhesion between the nanotubes and polymer chains because of the defects, which in turn causes an enhancement in the transverse Young's modulus and the transverse and longitudinal shear moduli of the composites. The simulation results on intermolecular interaction between Thrower–Stone–Wales defects and surrounding species can be used in macroscopic design of carbon nanotube- and graphene-based polymer composites. A semi-empirical approach was used to determine the interfacial shear strength of graphene oxide polymer composites by combining experiments with finite element modeling [12]. The study is important for designing of composites with nano-scale reinforcements such as graphenes and carbon nanotubes.

Thermal properties of carbon nanotube- and graphene-based nanocomposites were explored in Refs. [13–15]. Molecular simulations were used in Ref. [13] to examine the thermal conductance at graphene–matrix interfaces. The results show that the interfacial thermal conductance strongly depends on the mode of heat transfer. If heat enters graphene from one side of its basal plane and leaves it through the other side, the corresponding interfacial thermal conductance is large. However, if heat enters graphene from both sides of the plane and leaves it from a location far from the plane then the corresponding interfacial thermal conductance is small. These results are worthwhile in the optimal design of graphene-based thermal nanocomposites. A finite element model was developed by Safdari and Al-Haik [14] to estimate the thermal conductivities of hybrid carbon nanotube/graphite nanoplatelet/epoxy nanocomposites by taking into account the particle aggregation and deformation defects. The computational study suggests that the hybrid polymer nanocomposites outperform their single-nanofiller counterpart configurations. Mortazavi et al. [15] presented a multi-scale scheme using molecular dynamics and finite element method for evaluating the effective thermal conductivity of graphene/epoxy nanocomposites. The effect of formation of covalent bonds between graphenes and epoxy atoms on the effective thermal conductivity of nanocomposites has been also explored. The modeling results suggest that formation of covalent bonds between graphene and epoxy atoms slightly reduces the effective thermal conductivity of nanocomposites. Comparison between the multi-scale modeling results with experiments confirms the validity of the proposed multi-scale scheme in the evaluation of thermal conduction of polymer nanocomposites.

We hope you enjoy this selection of recent papers from *Carbon*, which we feel illustrates the power and promise of simulation and computation in carbon science and technology.

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