



## Guest editorial

## Special issue on nanocomposites

Thirteen articles comprise this special issue. They are arranged in a progression, from studies of the mechanics of individual nanostructures through small assemblies to nanocomposites, culminating in studies that draw on bio-inspiration or that address bio-composites. The main function of scientific research is to generate knowledge. I hope interest is sufficiently whetted by the brief description of each article that follows that each will be read in depth.

Various techniques to perform mechanical testing of single nanofibers are addressed in “Mechanical Characterization of Nanofibers – A Review” by Tan and Lim. Nanofibers can be made from different materials such as polymers, carbon, or ceramics, and be used for a wide range of applications such as tissue engineering, filter media and as reinforcements in composites. As these nanofibers are often subjected to physical stresses and strains that may result in permanent deformation or even failure, their mechanical properties need to be characterized. This paper reviews a variety of experimental techniques for the mechanical characterization of single nanofibers. These include tensile, bend, and indentation tests done at the nanoscale. The challenges involved in performing such nanoscale testing, current limitations, and future trends are also discussed.

The “Mechanics of Crystalline Boron Nanowires” is presented by Ding, Calabri, Chen, Kohlhaas, and Ruoff. Tensile testing and mechanical resonance methods were used to explore the elastic modulus and fracture strength of single crystal boron nanowires. The complicating effects of the presence of an oxide layer coating, specimen misalignment and imperfect boundary conditions on the determination of the mechanical properties of such nanowires are also discussed.

In “Flexural Deflection as a Measure of van der Waals Interaction Forces in the CNT Array,” Pipes, Hubert, Salvetat, and Zalamea show that the flexural stiffness of the hexagonal carbon nanotube (CNT) array directly correlates with the magnitude of the shearing traction between the individual CNT’s and thereby provides a convenient measurement of van der Waals forces acting in such arrays. Model predictions are combined with the experimental re-

sults of Salvetat et al. to determine the magnitude of the maximum shearing traction due to van der Waals forces in each of the arrays.

Coffin, Carlsson, and Pipes examine the energy density and the forces required to separate nanoropes into individual nanotubes by studying both the dilatation separation of arrays and the peeling of a pair of carbon nanotubes in “On the Separation of Carbon Nanotubes”. The energy of separation for the dilatation mechanism was shown to be a strong function of the array size with a significantly different energy density necessary to separate an array of three CNT’s as compared to separation of a large array.

In “Nanotube Mechanics – Recent progress in Shell Buckling Mechanics and Quantum Electromechanical Coupling,” Waters, Guduru, and Xu present their recent studies of the external microscopic and internal quantum mechanical responses of nanotubes to excess mechanical loading and electrical charging, providing thereby a basis for establishing an understanding of the uniaxial compression buckling behavior, and the dimensional change with charge injection of the nanotubes. Despite advances in modeling of the buckling behavior of nanotubes, experimental progress has been limited because of the difficulties in properly configuring the nanotubes for compressive loading. Here, buckling studies are enabled by fabricating nanotubes with an alumina template, yielding a uniform array of vertically oriented nanotubes extruding out of the template. Separately, Raman spectroscopy was used to probe the dimensional (bond length) change of the nanotubes under excess charge loading, after their release from the template. The shift of a strong and sharp enough G-band peak, thanks to the great uniformity and aggregation of the nanotubes, was monitored while increasing electron (or hole) concentration in excess of the equilibrium value. The Raman peak (phonon frequency) shift is a direct measure of the bond length (or strain) variation as a result of charge injection. These experiments when compared to theory, address the issue of whether quantum effects play a role in electro-mechanical coupling in nanotubes.

It is now well known that deformation in single-phase nanograin metals can exhibit high strength and hardness

but can also be susceptible to faster creep and microstructural coarsening at moderate temperatures. Nanoscale particulate composites may provide additional stiffness and strength while inhibiting undesirable deformation modes. To begin probing the prospects of nanoscale particulate composites, Ward, Qi, and Curtin have studied the deformation of model Al–Si nanocomposites via molecular dynamics, in “Aluminum–Silicon Interfaces and Nanocomposites: A Molecular Dynamics Study”. This preliminary study includes an in-depth study of fracture of interfaces, and the role that such interfaces play in deformation of Al–Si composites and suppression of both grain sliding and Al dislocation plasticity mechanisms typical of the single-phase material, as well as their role in the strength of such composites. This paper indicates that nanoscale metal-ceramic composites can provide enhanced properties and modify deformation mechanisms, and are amenable to nanostructure engineering.

An ongoing challenge in design of polymer nanocomposites to achieve their potential is understanding the complex interactions of nanoparticle chemistry, morphology and dispersion with the host matrix material. In “Reinforcement Mechanisms in MWCNT-filled Polycarbonate” by Eitan, Fisher, Andrews, Brinson, and Schadler, the load transfer mechanisms between nanotubes and matrix are investigated by Raman Spectroscopy. It is found that load transfer is improved by appropriate functionalization of the nanotubes to increase the interfacial bonding strength between them and the polymer matrix. The cause of this improved load transfer ability is shown to lie in the formation of a significant interphase layer of polymer of altered mobility near the nanotubes. Micromechanical analysis of the composite indicates that when the non-load bearing inner tubes of the MWNTs are accounted for, the mechanical properties are significantly enhanced by these altered polymer domains, which thus provide an important, unique, additional reinforcement mechanism for nano-filled composites.

Shim, Starkovich, and Kotov describe the application of the layer-by-layer assembly (LBL) method to the preparation of composites from vapor-grown carbon nanofibers (VGCFs), as presented in “Multilayer Composites from Vapor-Grown Carbon Nano-Fibers”. Besides the advantages of low cost, mass production, and relatively small impurity concentrations, VGCFs have convenient tubular morphology. Using the LBL film deposition method free-standing polymer composite films with very high loadings of VGCFs were successfully prepared. Combined with the permeable nature of polyelectrolyte multilayers, these layered composites may find use as smart materials with release-on-command functionality, which requires considerable mechanical strength and thermal and/or electrical conductivity. Their applications may include biological implants, anticorrosion coatings, and thermal/electrical interface materials.

The “Processing of Expanded Graphite Reinforced Polymer Nanocomposites,” is described and discussed by

Yasmin, Luo, and Daniel. It was found that properties of the fabricated nanocomposites depend on the processing method. Specific methods evaluated include direct, sonication, shear, and combined sonication and shear methods. Both sonication and shear mixing techniques produced exfoliation and dispersion of nanosheets. Increased sonication time improves the properties of the nanocomposite up to a point, but excessive sonication degrades them by inducing early polymerization of the matrix. The processing method had a strong influence on elastic modulus enhancement with the combined sonication/shear method producing the highest modulus.

Yu, Hu, Bekyarova, Itkis, Gao, Zhao, and Haddon focus on the dispersion of the single-walled carbon nanotubes (SWNTs) and the optimization of the interfacial interaction with the polyimide matrix in “Incorporation of Highly Dispersed Single Walled Carbon Nanotubes in a Polyimide Matrix”. They report the development of a novel strategy to disperse SWNTs in composites by making use of individual SWNTs and in situ polymerization. The debundling of SWNTs is achieved and AFM images show that the majority of the SWNTs are in the form of individual nanotubes. In situ polymerization with dispersions of individual SWNTs results in a composite film with good optical, and enhanced thermal and electrical properties. The incorporation of homogeneously dispersed individual SWNTs leads to a significant increase of the mechanical properties of SWNT–polyimide composite films.

In nature, many organisms have evolved elegant strategies for controlling the organic/inorganic interface. In the paper by Fan and Messersmith entitled “Surface-initiated Polymerization from TiO<sub>2</sub> Nanoparticle Surfaces through a Biomimetic Initiator: A New Route toward Polymer–matrix Nanocomposites,” the authors report a new strategy for surface initiated polymerization of organic polymers from inorganic nanoparticles. A new bifunctional initiator was developed that mimics DOPA, a key adhesive amino acid found in mussel adhesive proteins. The DOPA mimetic initiator was adsorbed onto the TiO<sub>2</sub> nanoparticle surfaces to provide an anchor for surface-initiated atom transfer radical polymerization from the particle surface. The properties of organic/inorganic interfaces in many conventional composites are susceptible to water absorption, and the use of such adhesive strategies may lead to improved organic/inorganic interfacial properties in composites employed in both wet and dry environments.

Organisms in nature are often faced with the task to build strong composites from abundant but low quality raw materials. The solution often lies in implementing nanocomposites with many orders of structural hierarchy. In the article “Hierarchical Interconnections in the Nanocomposite Material Bone: Fibrillar Cross-links Resist Fracture on Several Length Scales,” Fantner, Rabinovich, Schitter, Thurner, Kindt, Finch, Weaver, Golde, Morse, Lipman, Rangelow and Hansma describe fracture resisting schemes used in the multi-constituent bio-composite material bone. Based on the arrangement of bone constituents

from the nanoscopic to the microscopic scale, several types of filaments and cross links are discussed that resist the propagation of micro-cracks. These mechanisms contribute to the strength of the nanocomposite built from proteins and hydroxy apatite crystals.

Elastic properties including Young's modulus, shear modulus and Poisson's ratio of the mineral–protein nanostructure of bone have been addressed in the paper “Elastic Properties of Nanocomposite Structure of Bone” by Ji and Gao. Bone, a nanocomposite material consisting primarily of mineral and protein, exhibits superior mechanical properties and complex hierarchical structures. It is a both a challenge and a valuable endeavor to relate the macroscopic properties of bone to its hierarchical microstructures that start from the nanoscale. The authors show, through FEM calculations and simple analytical models to evaluate

the elastic properties of the mineral–protein nanostructure of bone, that the elastic properties of bone can be highly anisotropic at the nanoscale. An open question is how these nanoscale properties are related to the macroscopic properties of bone tissue via many levels of structural hierarchy.

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