
Computer Code for Nanostructure Simulation

John H. Glenn Research Center, Cleveland, Ohio

Due to their small size, nanostructures can have stress and thermal gradients that are larger than any macroscopic analogue. These gradients can lead to specific regions that are susceptible to failure via processes such as plastic deformation by dislocation emission, chemical debonding, and interfacial alloying.

A program has been developed that rigorously simulates and predicts optoelectronic properties of nanostructures of virtually any geometrical complexity and material composition. It can be used in simulations of energy level structure, wave functions, density of states of spatially configured phonon-coupled electrons, excitons in quantum dots,

quantum rings, quantum ring complexes, and more. The code can be used to calculate stress distributions and thermal transport properties for a variety of nanostructures and interfaces, transport and scattering at nanoscale interfaces and surfaces under various stress states, and alloy compositional gradients.

The code allows users to perform modeling of charge transport processes through quantum-dot (QD) arrays as functions of inter-dot distance, array order versus disorder, QD orientation, shape, size, and chemical composition for applications in photovoltaics and physical properties of QD-based biochemical sensors. The code can be used to study the hot exciton formation/relation dynamics in ar-

rays of QDs of different shapes and sizes at different temperatures.

It also can be used to understand the relation among the deposition parameters and inherent stresses, strain deformation, heat flow, and failure of nanostructures.

This work was done by Igor Filikhin and Branislav Vlahovic of North Carolina Central University for Glenn Research Center. Further information is contained in a TSP (see page 1).

Inquiries concerning rights for the commercial use of this invention should be addressed to NASA Glenn Research Center, Innovative Partnerships Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-18414-1.

Functionalizing CNTs for Making Epoxy/CNT Composites

Lyndon B. Johnson Space Center, Houston, Texas

Functionalization of carbon nanotubes (CNTs) with linear molecular side chains of polyphenylene ether (PPE) has been shown to be effective in solubilizing the CNTs in the solvent components of solutions that are cast to make epoxy/CNT composite films. (In the absence of solubilization, the CNTs tend to clump together instead of becoming dispersed in solution as needed to impart, to the films, the desired CNT properties of electrical conductivity and mechanical strength.) Because the PPE functionalizes the CNTs in a non-covalent manner, the functionalization does not damage the CNTs. The function-

alization can also be exploited to improve the interactions between CNTs and epoxy matrices to enhance the properties of the resulting composite films.

In addition to the CNTs, solvent, epoxy resin, epoxy hardener, and PPE, a properly formulated solution also includes a small amount of polycarbonate, which serves to fill voids that, if allowed to remain, would degrade the performance of the film. To form the film, the solution is drop-cast or spin-cast, then the solvent is allowed to evaporate.

This work was done by Jian Chen and Ramasubramaniam Rajagopal of Zyvex Corp.

for Johnson Space Center. For further information, contact the Johnson Commercial Technology Office at (281) 483-3809.

In accordance with Public Law 96-517, the contractor has elected to retain title to this invention. Inquiries concerning rights for its commercial use should be addressed to:

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Refer to MSC-23719-1, volume and number of this NASA Tech Briefs issue, and the page number.

Improvements in Production of Single-Walled Carbon Nanotubes

Continuous mass production in fluidized-bed reactors now appears feasible.

Lyndon B. Johnson Space Center, Houston, Texas

A continuing program of research and development has been directed toward improvement of a prior batch process in which single-walled carbon nanotubes are formed by catalytic disproportionation of carbon monoxide in a fluidized-bed reactor. The overall effect of the improvements has been to make progress toward converting the

process from a batch mode to a continuous mode and to scaling of production to larger quantities. Efforts have also been made to optimize associated purification and dispersion post processes to make them effective at large scales and to investigate means of incorporating the purified products into composite materials. The ultimate purpose of the

program is to enable the production of high-quality single-walled carbon nanotubes in quantities large enough and at costs low enough to foster the further development of practical applications.

The fluidized bed used in this process contains mixed-metal catalyst particles. The choice of the catalyst and the operating conditions is such that the yield of