
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

single-walled carbon nanotubes, relative to all forms of carbon (including carbon fibers, multi-walled carbon nanotubes, and graphite) produced in the disproportionation reaction is more than 90 weight percent. After the reaction, the nanotubes are dispersed in various solvents in preparation for end use, which typically involves blending into a plastic, ceramic, or other matrix to form a composite material.

Notwithstanding the batch nature of the unmodified prior fluidized-bed process, the fluidized-bed reactor operates in a continuous mode during the process. The operation is almost entirely automated, utilizing mass flow controllers, a control computer running software specific to the process, and other equipment. Moreover, an important inherent advantage of fluidized-bed reactors in general is that solid particles can be added to and re-

moved from fluidized beds during operation. For these reasons, the process and equipment were amenable to modification for conversion from batch to continuous production.

The improvements include the following:

- A provision has been made for continuous addition of catalyst particles by entraining them in a stream of helium that is fed into the reactor.
- Progress has been made toward implementation of a purification/suspension post-process.
- Progress has also been made toward implementation of an alternative purification process that involves the use of hydrofluoric acid.
- A post-purification drying method was invented. This method increases the probability of success of subsequent efforts to re-disperse lyophilized samples of purified product material.

- Techniques of *in-situ* polymerization were explored. The findings may lead to development of strong, lightweight carbon-nanotube/polymer composites.

This work was done by Leandro Balzano and Daniel E. Resasco of SouthWest Nano Technologies, Inc., for Johnson Space Center. For more information, see www.swnano.com.

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-23706-1, volume and number of this NASA Tech Briefs issue, and the page number.

Progress Toward Sequestering Carbon Nanotubes in PmPV

Lyndon B. Johnson Space Center, Houston, Texas

A report reopens the discussion of "Sequestration of Single-Walled Carbon Nanotubes in a Polymer" (MSC-23257), *NASA Tech Briefs*, Vol. 31, No. 12 (December 2007), page 38. To recapitulate: Sequestration of single-walled carbon nanotubes (SWNTs) in molecules of poly(*m*-phenylenevinylene-co-2,5-dioctyloxy-*p*-phenylenevinylene) [PmPV] is a candidate means of promoting dissolution of single-walled carbon nanotubes (SWNTs) into epoxies for making strong, lightweight epoxy-matrix/carbon-fiber composite materials. Bare SWNTs cannot be incorporated because they are not soluble in epoxies. One can render SWNTs soluble by chemically at-

taching various molecular chains to them, but such chemical attachments weaken them. In the present approach, one exploits the tendency of PmPV molecules to wrap themselves around SWNTs without chemically bonding to them. Attached to the backbones of the PmPV molecules are side chains that are soluble in, and chemically reactive with, epoxy precursors, and thus enable suspension of SWNTs in epoxy precursors. At time of the cited prior article, there had been only partial success in functionalizing the side chains to make them sufficiently soluble and reactive. The instant report states that a method of functionalization has been developed.

This work was done by Richard A. Bley of Eltron Research, Inc. for Johnson Space Center. Further information is contained in a TSP (see page 1).

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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