



## Switching and Rectification in Carbon-Nanotube Junctions

Research shows promise for nanoscale electronic devices.

Ames Research Center, Moffett Field, California

Multiterminal carbon-nanotube junctions are under investigation as candidate components of nanoscale electronic devices and circuits. Three-terminal “Y” junctions of carbon nanotubes (see Figure 1) have proven to be especially interesting because (1) it is now possible to synthesize them in high yield in a controlled manner and (2) results of preliminary experimental and theoretical studies suggest that such junctions could exhibit switching and rectification properties.

Following the preliminary studies, current-versus-voltage characteristics of a number of different “Y” junctions of single-wall carbon nanotubes connected to metal wires were computed. Both semiconducting and metallic nanotubes of various chiralities were considered. Most of the junctions considered were symmetric. These computations involved modeling of the quantum electrical conductivity of the carbon nanotubes and junctions, taking account of such complicating factors as the topological defects (pentagons, heptagons, and octagons) present in the hexagonal molecular structures at the junctions, and the effects of the nanotube/wire interfaces. A major component of the computational approach was the use of an efficient Green’s function embedding scheme.

The results of these computations showed that symmetric junctions could be expected to support both rectification and switching. The results also showed that rectification and switching properties of a junction could be expected to depend strongly on its symmetry and, to a lesser degree, on the chirality of the nanotubes. In particular, it was found that a zigzag nanotube branching at a symmetric “Y” junction could exhibit either perfect rectification or partial rectification (asymmetric current-versus-voltage characteristic, as in the example of Figure 2). It was also found that an asymmetric “Y” junction would not exhibit rectification.

*This work was done by Deepak Srivastava of Ames Research Center; Antonis N. An-*

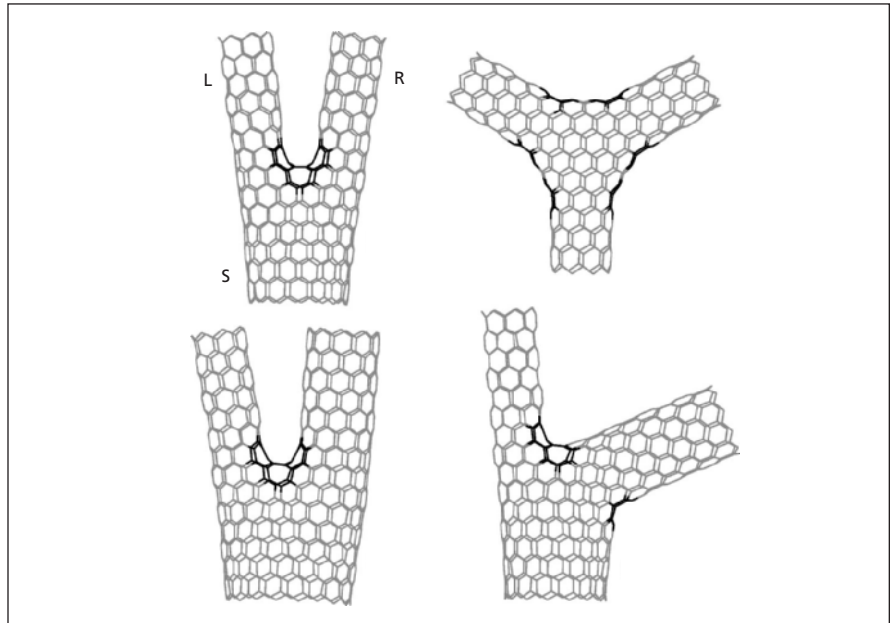


Figure 1. **Symmetric and Asymmetric Carbon-Nanotube “Y” Junctions** have been studied experimentally and theoretically as candidate electronic switches and rectifiers.

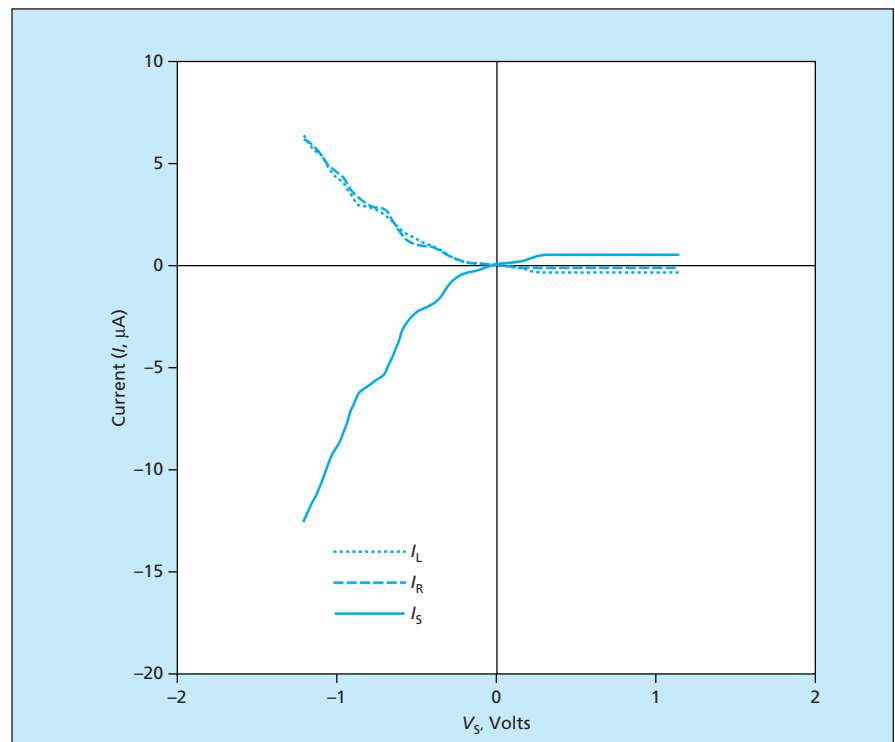


Figure 2. These **Current-Versus-Voltage Characteristics** were computed for the three branches of the symmetric junction depicted in the upper left part of Figure 1, with zero potential applied to branches L and R and a potential  $V_S$  applied to branch S.

driotis of the Institute of Electronic Structure and Laser, Foundation for Research and Technology — Hellas; Madhu Menon of the University of Kentucky; and Leonid Cher-

nozatonskii of the Institute of Biochemical Physics of the Russian Academy of Sciences. Further information is contained in a TSP (see page 1).

Inquiries concerning rights for the commercial use of this invention should be addressed to the Patent Counsel, Ames Research Center, (650) 604-5104. Refer to ARC-15092.

## Scandia-and-Yttria-Stabilized Zirconia for Thermal Barriers

**These compositions offer thermal stability greater than that of yttria-stabilized zirconia.**

*John H. Glenn Research Center, Cleveland, Ohio*

Zirconia stabilized with both scandia and yttria in suitable proportions has shown promise of being a superior thermal-barrier coating (TBC) material, relative to zirconia stabilized with yttria only. More specifically, a range of compositions in the zirconia/scandia/yttria material system has been found to afford increased resistance to deleterious phase transformations at temperatures high enough to cause deterioration of yttria-stabilized zirconia.

Yttria-stabilized zirconia TBCs have been applied to metallic substrates in gas turbine and jet engines to protect the substrates against high operating temperatures. These coatings have porous and microcracked structures, which can accommodate strains induced by thermal-expansion mismatch and thermal shock. The longevity of such a coating depends upon yttria as a stabilizing additive that helps to maintain the zirconia in an yttria-rich, so-called “non-transformable” tetragonal crystallographic phase, thus preventing transformation to the monoclinic phase with an associated deleterious volume

change. However, at a temperature greater than about 1,200 °C, there is sufficient atomic mobility that the equilibrium, transformable zirconia phase is formed. Upon subsequent cooling, this phase transforms to the monoclinic phase, with an associated volume change that adversely affects the integrity of the coating.

Recently, scandia was identified as a stabilizer that could be used instead of, or in addition to, yttria. Of particular interest are scandia-and-yttria-stabilized zirconia (SYSZ) compositions of about 6 mole percent scandia and 1 mole percent yttria, which have been found to exhibit remarkable phase stability at a temperature of 1,400 °C in simple aging tests. Unfortunately, scandia is expensive, so that the problem becomes one of determining whether there are compositions with smaller proportions of scandia that afford the required high-temperature stability. In an attempt to solve this problem, experiments were performed on specimens made with reduced proportions of scandia. The criterion used to judge

these specimens was whether they retained the “non-transformable” tetragonal phase after a severe heat treatment of 140 hours at 1,400 °C. On the basis of this criterion and limited data, the locus of favored compositions is specified as follows: mole percent of yttria =  $8.55 - 1.5 \times$  (mole percent of scandia) between and near the compositional end points of

- 4.9 mole percent scandia and 1.2 mole percent yttria and
- 3.7 mole percent scandia and 3.0 mole percent yttria.

In addition, it appears that a composition of  $\approx 3$  mole percent scandia and  $\approx 2.5$  mole percent yttria may confer the desired phase stability at 1,400 °C.

*This work was done by Derek Mess of Cambridge Microtech, Inc., 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, Commercial Technology Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-16789.*

## Environmentally Safer, Less Toxic Fire-Extinguishing Agents

**Water droplets would be microencapsulated in flame-retardant polymers.**

*John F. Kennedy Space Center, Florida*

Fire-extinguishing agents comprising microscopic drops of water microencapsulated in flame-retardant polymers have been proposed as effective, less toxic, non-ozone-depleting, non-global-warming alternatives to prior fire-extinguishing agents. Among the prior fire-extinguishing agents are halons (various halocarbon fluids), which are toxic and contribute both to depletion of upper-atmospheric ozone and to global warming. Other prior fire-extinguishing agents are less toxic and less environmentally harmful but, in comparison

with halons, are significantly less effective in extinguishing fires.

The proposal to formulate new water-based agents is based on recent success in the use of water mist as a fire-suppression agent. Water suppresses a flame by reducing the flame temperature and the concentration of oxygen available for the combustion process. The temperature is reduced because the water droplets in the mist absorb latent heat of vaporization as they evaporate. The concentration of oxygen is reduced because the newly generated

water vapor displaces air.

Unfortunately, water mists are difficult to produce in confined spaces and can evaporate before they reach the bases of flames. The proposal addresses both of these issues: The proposed fire-extinguishing agents would be manufactured in microencapsulated form in advance, eliminating the problem of generating mists in confined spaces. Because of the microencapsulation, the droplets would not evaporate until exposed directly to the heat of flames. In addition, the proposal calls for the in-