For submission to the MRS 2002 Fall meeting, to be held in Boston, Massachusetts, December 2-6, 2002
(http://www.mrs.org/meetings/fall2002/cfp/)

Field Emission Properties of BN/C and BN@C hybrids

V. Meunier[1], C. Roland[2], J. Bernholc[2], T. Zacharia[1], and M. Buongiorno Nardelli[1, 2]

[1]Oak Ridge National Laboratory, Oak Ridge, Tennessee
[2]North Carolina State University, Raleigh, North Carolina

The discovery of carbon (C) nanotubes as a material with outstanding mechanical and electrical properties has led to a quest for other novel graphene-based structures with technologically desirable properties. The closely related boron (B) nitride (N) nanotubes and mixed BNC systems have electronic properties that are complementary to pure carbon nanotubes. For example, BN nanotubes posses a non-zero spontaneous polarization that makes them strong pyro- and piezoelectics. The polarized B-N bond gives rise to important effects in the electronic properties of BN-doped carbon nanotubes. BNC hybrids are basically found in two distinct configurations: a quasi 1D BN/C heterostructure or a 2D BN@C bi-walled system. In the former, the BN and C phases are covalently joined while they are segregated in the latter.

In this paper, we show that the presence of BN allows for an important increase of the field emission properties at the carbon tip. The intrinsic electric field associated with the B-N bond indeed induces a substantial reduction in the work function at the carbon tip. The change in the work function greatly improves the field emission properties, since the decrease in the work function exponentially increases the current density, compared to a pure carbon nanotube. Using state-of-the-art large-scale *ab initio* calculations, we show that this effect is present in both BN@C and BN/C systems. While the improvement is limited in the coaxial geometry, the current density is predicted to increase by up to 2 orders of magnitude in the BN/C systems.

Research sponsored by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research; U.S. Department of Energy, under Contract No. DE-AC05-00OR22725 with UT-Battelle, LLC.