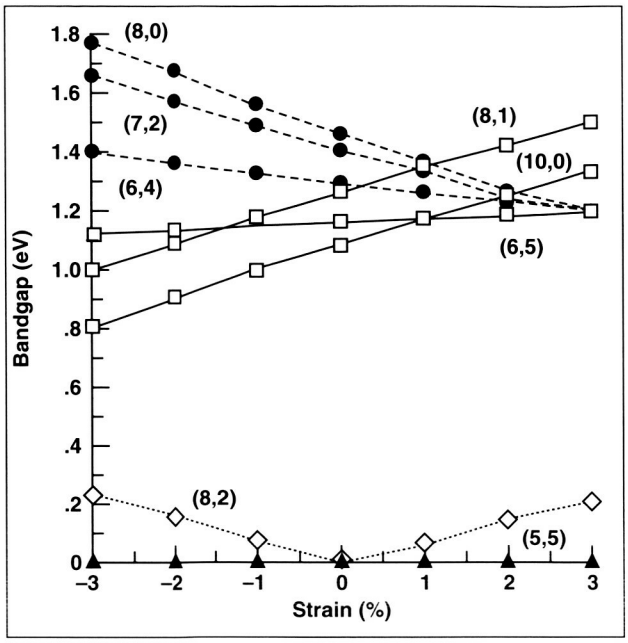

Fig. 2. Band gap versus tensile strain: for semiconducting tubes, the sign of slope of band gap versus strain depends only on the value of (n – m) mod 3 values of 1, -1 and 0, respectively.

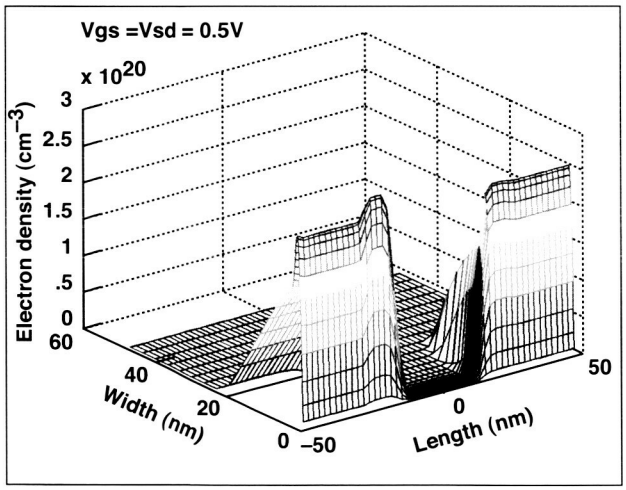

Fig. 3. Self-consistently calculated charge density when the gate and drain bias is equal to 0.5 V. The grid spacing is about an Angstrom near the gate (x = 0 nm), and 10 times larger near the substrate (x = 120 nm). The x-axis is perpendicular to the gate (from gate to substrate) and the y-axis is along the transport direction (from source to drain). X and Y are in units of nm, and density is in units of cm^{-3}.

Plasticity and Kinky Chemistry of Carbon Nanotubes

Deepak Srivastava, Fedor Dzegilenko

Since their discovery in 1991, carbon nanotubes have been the subject of intense research interest based on early predictions of their unique mechanical, electronic, and chemical properties. Materials with the predicted unique properties of carbon nanotubes are of great interest for use in future generations of aerospace vehicles. For their structural properties, carbon nanotubes could be used as reinforcing fibers in ultralight multifunctional composites. For their electronic properties, carbon nanotubes offer the potential of very high-speed, low-power computing elements, high-density data storage, and unique sensors. In a continuing effort to model and predict the properties of carbon nanotubes, Ames accomplished three significant results during FY99. First, accurate values of the nanomechanics and plasticity of carbon nanotubes based on quantum molecular dynamics simulations were computed. Second, the concept of mechanical deformation catalyzed—kinky—chemistry as a means to control local chemistry of nanotubes was discovered. Third, the ease of nano-indentation of silicon surfaces with carbon nanotubes was established.

The elastic response and plastic failure mechanisms of single-wall nanotubes were investigated by means of quantum molecular dynamics simulations. Working with researchers from Stanford University and the University of Kentucky, it was found that the elastic limit of thin carbon nanotubes under axial compression is significantly lower than earlier predictions based on classic molecular dynamics investigations. A novel mechanism of nanoscale plasticity is observed in which bonding geometry collapses from a graphitic to a localized diamond-like reconstruction. Figure 1 shows a compressed nanotube collapsed near the two edges by plastic deformation. The bonding geometry shown in figure 1(b) reveals a diamond-like structure at the location of the collapse. The computed critical stress (approximately 153 gigapascals) for the collapse and the shape of the resulting deformation are in good agreement with recent experimental observations of compressed nanotubes in polymer composites. These

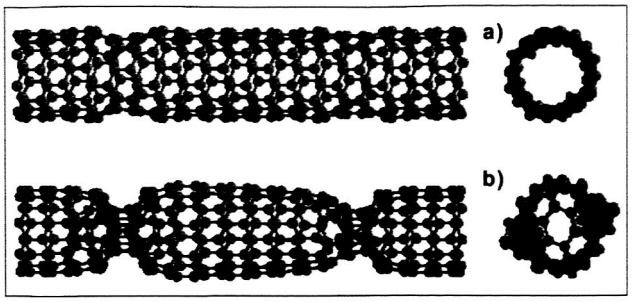

Fig. 1. (a) Compressed nanotube collapsed near the two edges by plastic deformation. (b) A diamond-like structure at the location of the collapse.

results are a first step in the accurate characterization of isolated nanotubes for their potential application in ultralight structural composites for aerospace applications.

The relationship between mechanical deformation and chemical reactivity (mechano- or kinky-chemistry) of carbon nanotubes was investigated in a collaborative effort between Ames, North Carolina State University, and the University of Washington at St. Louis. The sidewalls of pure nanotubes are relatively inert, whereas the end-caps are reactive. However, for many applications selective sidewall functionalization or reactivity of carbon nanotubes is highly desired. It is shown that such reactivity could be enhanced and controlled by mechanical deformations. When a mechanically twisted or kinked tube is exposed to an environment of reactant, the reactant specifically functionalizes (adsorbs) or etches the twist or kink. Figure 2(a) shows a twisted nanotube that has flattened into a ribbon-like structure with sharp edges. Figure 2(b) shows the preferential adsorption of atomic H at the strained edges of the twisted nanotube. For the first time, computational prediction of the kinky chemistry of nanotubes has been experimentally verified in a proof-of-principle experiment at University of Washington at St. Louis.

Indentation of diamond and silicon surfaces with carbon nanotubes used as atomic force microscope (AFM) tips was simulated. Indentation of a diamond surface by a nanotube causes buckling and collapse of the tube. However, a nanotube very easily indents a silicon surface. Thus, this technique can be used for making nanoscale holes on silicon surfaces with potential applications in high-density data storage, or nanolithography of silicon surfaces for electronics applications.

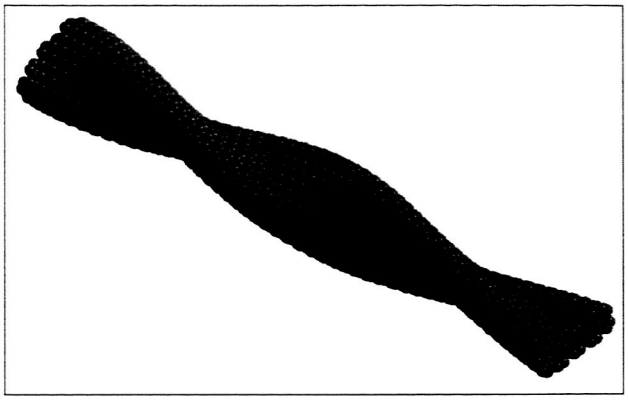

Fig. 2(a). Twisted nanotube that has flattened into a ribbon-like structure with sharp edges.

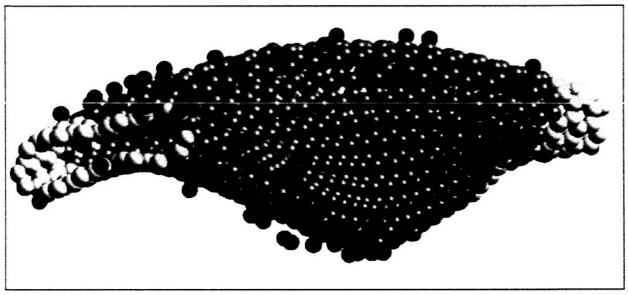

Fig. 2(b). Preferential adsorption of atomic H at the strained edges of the twisted nanotube.

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