SIMULATIONS OF TRANSPORT AND FIELD-EMISSION PROPERTIES OF MULTI-WALL CARBON NANOTUBES

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We present simulations of transport and field emission properties of multi-wall carbon nanotubes [1], by using a transfer-matrix methodology [2] for taking account of three-dimensional aspects of the potential-energy distribution. Band-structure effects result from the periodic repetition of a basic unit of the nanotubes and by using pseudopotentials [3] for the representation of carbon atoms.

The configuration considered for the transport simulations consists of (10,10) or (15,15) single-wall slots, which are used to introduce electrons in a single layer of a (5,5)@(10,10)@(15,15)@(20,20) multi-wall nanotube (see Fig. 1 for a representation of the junction between the nanotubes). The study focuses on the distance this electronic flux can cross before spreading significantly to neighboring layers. The results indicate that the layers of multi-wall nanotubes may be used as independent current conduction channels over distances that will be discussed.

Simulations of field emission from flat- or convex-terminated (5,5)@(10,10)@(15,15) nanotubes are presented (see Fig. 2 for a representation of the potential-energy distribution around the convex-terminated structure). The total-energy distributions exhibits features that are related to band-structure effects, to resonant states at the apex of the nanotubes and to standing waves in the structure. The calculations reveal that the emission properties of multi-wall nanotubes are better than those of their single-wall components, essentially because of a lower global polarizability of multi-wall structures. The consequences of closing the nanotubes, of saturating the dangling bonds by hydrogen and the efficiency of a photo-stimulation process to control the emission will be presented.

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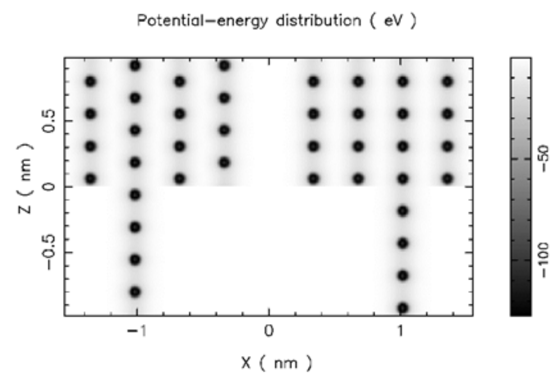

Figure 1: Potential-energy distribution at the jonction between a (15,15) single-wall slot and a (5,5)@(10,10)@(15,15)@(20,20) multi-wall nanotube.

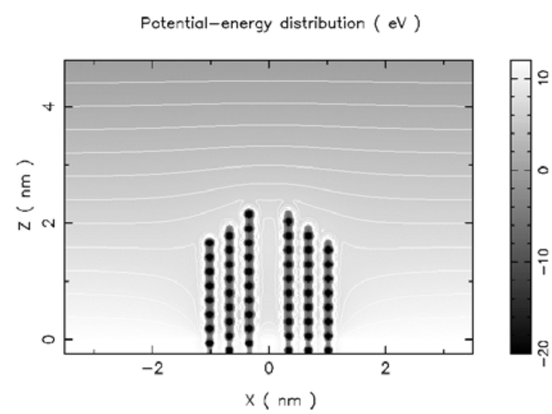

Figure 2: Potential-energy distribution around a convex-terminated (5,5)@(10,10)@(15,15) multi-wall nanotube, for a cathode-anode distance of 4.8 nm and a bias of 12 V.