Charge spreading effects during 3D tunneling through a supported carbon nanotube

Géza I. Márk*,†, László P. Biró*, Antal Koós*, Zoltán Osváth*, József Gyulai*, Ana M. Benito‡, Paul A. Thiry†, and Philippe Lambin†

*Research Institute for Technical Physics and Materials Science, H-1525 Budapest P.O.Box 49, Hungary, E-mail: mark@sunserv.kfki.hu
†Département de Physique, Facultés Universitaires Notre-Dame de la Paix 61, Rue de Bruxelles, B-5000 Namur, Belgium
‡Instituto de Carboquimica (CSIC), C/Miguel Luesma Castan 4 E-50015 Zaragoza, Spain

Abstract. Investigating the distribution of the scanning tunneling microscope (STM) current through a nanostructured material is a subject of great current interest. In this work, the transmission of an electron wave packet was calculated through a jellium potential model of a carbon nanotube under the tip of a STM. Snapshots of the full three-dimensional (3D) probability density of the wave packet enabled us to study in detail the tunneling event. The theory shows that the wave packet spreads along the nanotube while it tunnels through it and the nanotube-support tunneling channel is also extended along the direction of the tube as compared to the tip-nanotube channel which remains narrow. We demonstrate how can this spread explain the characteristics of the apparent height measured by STM of a nanotube crossing a step on graphite.

INTRODUCTION

The full three-dimensional (3D) transmission of electron wave packets (WPs) was calculated through a jellium potential model of a carbon nanotube (CNT) under the tip of a scanning tunneling microscope (STM). This work is an extension of our former two-dimensional (2D) calculations [1,2] where the tunneling process was only examined in the plane perpendicular to the CNT. The 2D approach is capable of explaining some important effects influencing STM and scanning tunneling spectroscopy (STS) results (tip-sample convolution [1], effect of the two tunnel gaps, ballistic vs. tunneling contact [2]), but it can not describe the consequences of the different dimensionality of the tip-CNT and CNT-support contacts.

CALCULATION METHOD AND RESULTS

The tunneling problem was regarded as a problem in potential scattering theory. In the present approach we used a simple jellium potential which does not take into account the atomic structure. At this level of approximation, all CNTs are metallic. The model system geometry used in our calculation is shown in the upper left panel of *Fig. 1.* The CNT is modeled by a cylinder of $0.5\,nm$ radius floating above the support plane at a distance of $0.335\,nm$. The STM tip is taken as a hyperboloid of $0.5\,nm$ apex radius. The chosen value [1] of $0.4\,nm$ for the tip-CNT tunnel gap is consistent with that estimated from the apparent geometric distortion of the CNT atomic lattice [3] seen in STM experiments.

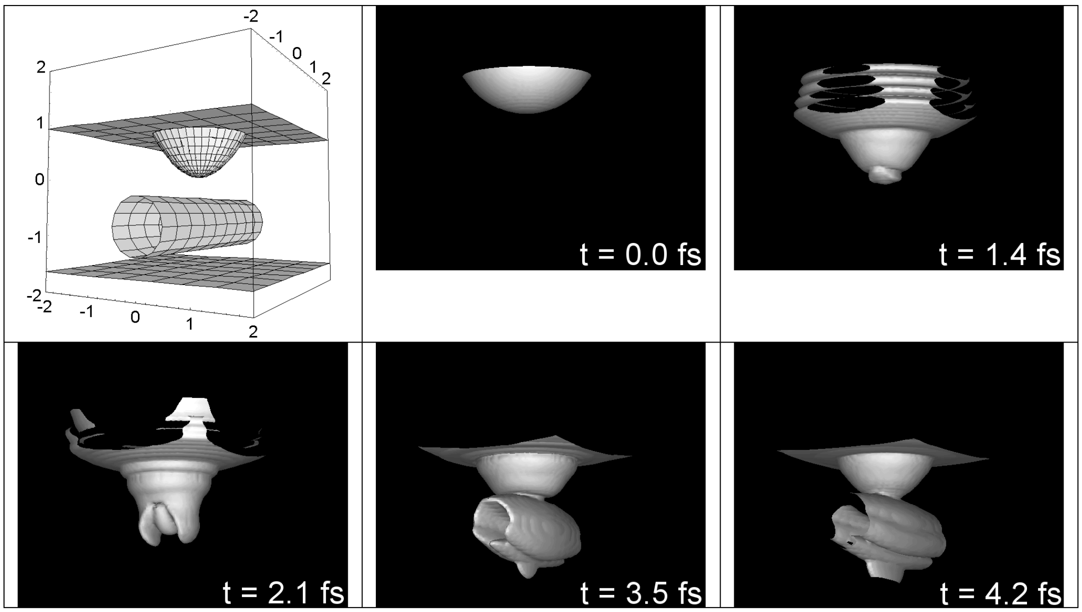

FIGURE 1. Time evolution of the probability density of the wave packet approaching the STM junction from the tip bulk and tunneling through the nanotube into the support. The upper left image is the model system used in the calculation. The labeled box is the presentation box. All dimensions are in nm. The subsequent images show snapshots of a constant probability density surface. This surface is clipped at the presentation box boundaries. See the text for details.

The time development of a Gaussian WP approaching the tunnel junction from inside of the tip bulk was calculated by numerically solving the time dependent 3D Schrödinger equation with the split time FFT method [1] The $\rho(x,y,z,t) = |\psi(x,y,z,t)|^2$ time dependent probability density function is visualized by snapshots of a constant density surface in *Fig. 1.* A computer animation showing the details of the tunneling process is available on the WEB [4].

In the panel $t = 0.0\,fs$ of *Fig. 1.* the initial WP is shown. The sphere surface is clipped at the upper boundary of the presentation box. At $t = 1.4\,fs$ the WP has already penetrated into the tip apex region. The part reflected back into the tip bulk forms interference patterns with the incoming wave. A fraction of the WP just begins to enter into the tip-CNT interface. At $t = 2.1\,fs$ the WP flows around the tube and simultaneously tunnels through it. The incoming and outgoing waves form interference patterns in the tip apex region. When the two WP parts (one moving on the left side and another on the right side of the tube) meet at the lowest point, standing wave patterns begin to form along the tube circumference. Subsequently the WP tunnels through the CNT-support junction and enters into the support surface (at $t = 3.5\,fs$). In the meantime the probability density is gradually spreading along the tube axis. At $t = 4.2\,fs$ the CNT-support tunnel channel begins to open along the tube axis.

DISCUSSION AND CONCLUSION

Our new 3D approach makes it for the first time possible to study the phenomenon of WP spreading along the CNT while tunneling through it. This spreading can explain the features of the STM image shown in *Fig. 2 (upper)*.

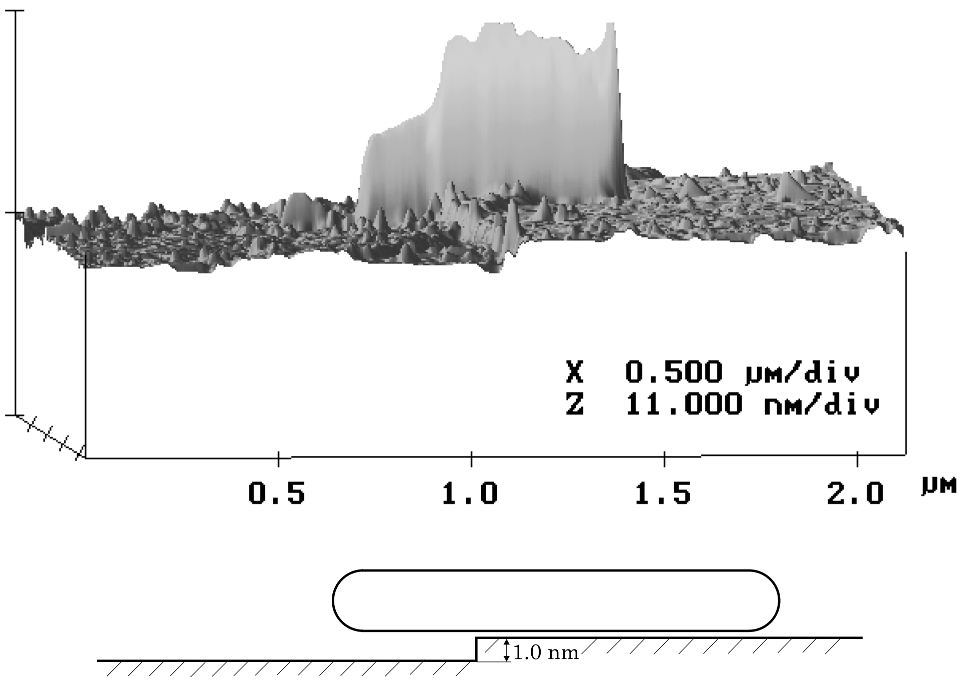

FIGURE 2. *(upper)* Constant current 3D STM image of a multiwall carbon nanotube crossing a step on the HOPG support surface. Note the gradual decrease of the apparent height of the tube section above the lower terrace. Also note the transition region at the step edge. *(lower)* Schematic model of the tube crossing the step.

A short and thick multiwall carbon nanotube (MWCNT) produced by the arc method in Zaragoza was found during constant current STM imaging being adsorbed on a step edge in such a way that part of the tube is protruding from the step edge. *Fig. 2 (lower)* is a schematic model of the MWCNT crossing the step.

The tube part above the lower terrace is floating above the HOPG surface at a distance of $1.3\,nm$. As revealed by TEM investigation of the MWCNTs these are compact structures with many layers and a narrow empty core. As shown by molecular mechanics calculations [5], due to their construction such multiwall structures behave like rigid objects. As a consequence, the short tube does not bend to make contact with the substrate on the lower terrace of the step. If bending to contact would occur, one should measure the same height value on the lower terrace as on the upper one which was contrary to the experimantal observation (see *Fig. 2*). The apparent height of the tube part above the higher terrace is constant (some noise is present) because of the translational symmetry along the tube. As seen in the 3D image, right at the step edge there is a transition region in the apparent height measured, the width of this region corresponds to the length over which the charge spreading takes place along the tube. When the step height is of the order of nanometers no tunneling can occur from the tube to the support. If the distance of the STM tip as measured from the step edge is larger than the lateral WP spreading length, the electrons can reach the support of the tube only after transport occurs along the tube. This explains the ohmic like decrease of the apparent height along the tube [6]. As a consequence, a more pronounced drop is found in the apparent height of the tube than the geometric height of the step in that part where the tube is not supported.

In conclusion the full 3D WP tunneling simulation is an useful tool in interpretating experimental data and predicting the likely behavior of nanodevices buit from carbon nanotubes, like CNTs crossing each other.

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