Full three-dimensional wave-packet dynamical calculations of STM images of nanotube Y-junctions

Géza I. Márk*, László P. Biró*, József Gyulai*, Zoltán Kónya†, 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
†Applied and Environmental Chemistry Department, University of Szeged H-6720 Szeged, Hungary
‡Département de Physique, Facultés Universitaires Notre-Dame de la Paix 61, Rue de Bruxelles, B-5000 Namur, Belgium

Abstract. Due to their geometry and asymmetric transport properties, carbon nanotube Y-junctions make it possible to create three-terminal nanoelectronic devices and fully nanoscale device networks. To understand the propagation of electron waves in these nanoscopic "wave guides", we have simulated the STM images of such systems by calculating the transversal propagation of electronic wave packets through an STM model. The STM tip acts as a local injection source, the variation of the probability density along the branches of the Y-junction gives information about the wave packet reflections and localized states.

INTRODUCTION

Single-wall carbon nanotubes (SWCNTs) offer a new route to the possible advances in the area of nanoscale devices. In molecular electronics devices made from three terminal nanotube junctions, the 3rd terminal could be used as a gate electrode. SWCNT "T-" and "Y-junctions" were first proposed theoretically [1,2] and later found experimentally by STM [3]. Recently, techniques for high-yield and reproducible production of Y-junctions were developed [4,5]. Their measured [5] asymmetric conductance were recently explained theoretically [6].

To explore the formation of the STM image of Y-junctions we have calculated the tunneling of three-dimensional (3D) electron wave packets (WPs) [7,8] through a jellium potential model of a supported Y-junction under the STM tip.

CALCULATION METHOD AND RESULTS

The tunneling problem was regarded as a problem in potential scattering theory. A simple jellium potential was used 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 Y-junction is modeled by three joined cylinders 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.

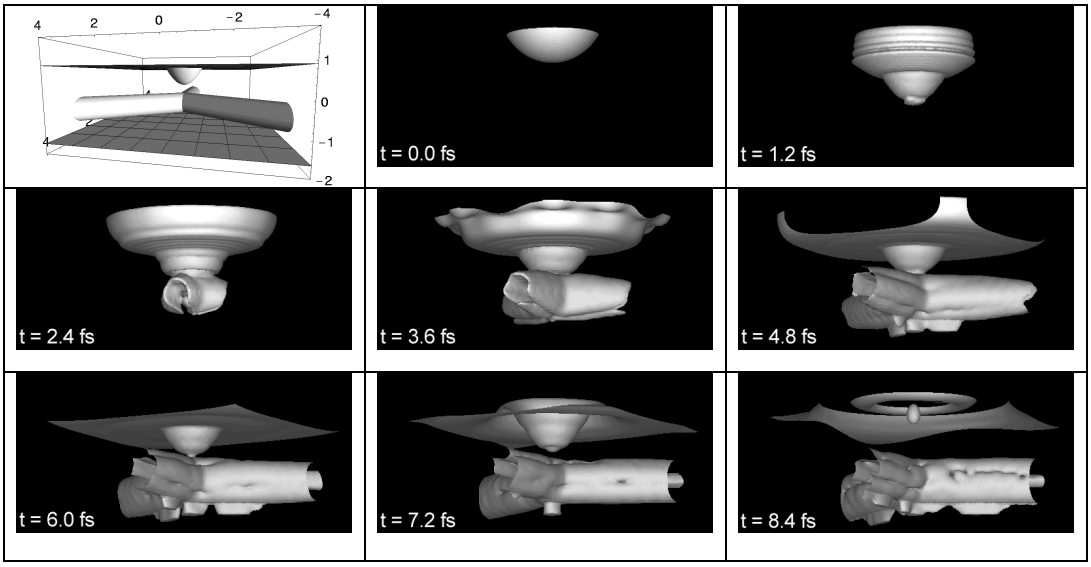

FIGURE 1. Time evolution of the probability density of the wave packet approaching the STM junction from the tip bulk and tunneling through the nanotube into the support. The upper left image is the model system used in the calculation. The labeled box is the presentation box. All dimensions are in *nm*. 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 the tip bulk was calculated by numerically solving the time dependent 3D Schrödinger equation with the split time FFT method [7] 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. Two tip positions were analyzed. In *Fig. 1.* the tip is above the center of the Y-junction while *Fig. 2.* shows a situation where the tip is displaced by $1.2\,nm$ along one of the branches.

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 $t = 1.2\,fs$ 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–Y interface. At $t = 2.4\,fs$ the WP flows around the star shaped junction of the three tubes 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 each sides of the tubes) meet at the lowest point, standing wave patterns begin to form along the circumference of the tubes (at $t = 3.6\,fs$). Subsequently the WP tunnels through the CNT-support junction and enters into the substrate (at $t = 4.8\,fs$). In the meantime the probability density is gradually spreading along the tube axis. Note that the shape of the Y-junction – support tunnel channel develops in time along a complex pattern. By around $t = 7.0\,fs$ most of the incoming WP is already reflected back into the tip bulk. Hence the structures seen in the tip region at the frames $t = 7.2\,fs$ and $t = 8.4\,fs$ show the WP parts tunneling back from the Y-junction to the tip.

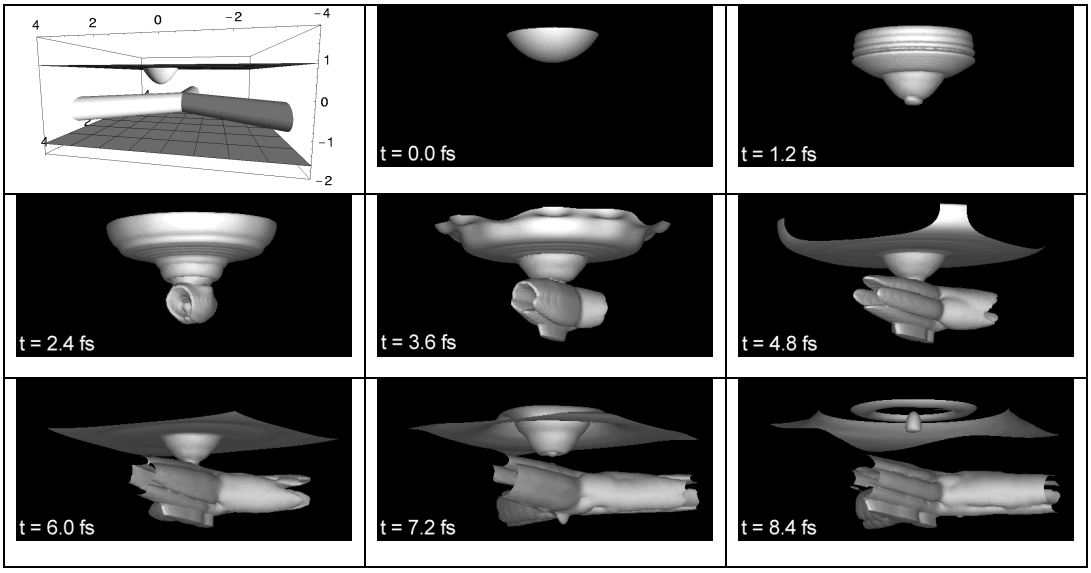

FIGURE 2. Time evolution of the probability density of the wave packet for the case of a tip displaced $1.2\,nm$ from the center along one of the branches. See the text for details.

In *Fig. 2.* the tip is displaced from the joining point along one of the branches. Hence the first part of the time development ($t = 0.0\,fs$, $t = 1.2\,fs$, and $t = 2.4\,fs$) shows the same features as for the case of a single CNT studied earlier [9,10]. However, when the part of the WP spreading along the tube in the direction of the center reaches the joining point it begins to split along the other two tubes (at $t = 3.6\,fs$).

The total probability of the WP flowing out from the tip apex is $4.63 * 10^{-4}$ for the tip above the center and $4.05 * 10^{-4}$ for the tip displaced by $1.2\,nm$.

DISCUSSION AND CONCLUSION

The present results are in agreement with experimental data [11] showing that when tunneling occurs in the vicinity of the junction through an all metallic Y-junction, no tunneling current maxima are to be expected. The 14 % difference in the calculated tunneling currents at the junction and on one of the branches should not produce a significant difference in the topographic STM images. A different behavior is expected for a mixed metal / semiconductor junction, which we are not able to consider with our present jellium modeling.

In conclusion the 3D WP tunneling simulation is an useful tool in interpretating experimental data and predicting the likely behavior of nanodevices built from carbon nanotubes, like Y-junctions.

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