Wave packet tunneling through an atomic pseudopotential model of a carbon nanotube

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Abstract. STM images of carbon nanotubes always contain the influence of both the geometrical and electronic structure. In our several former papers [1,2] we explored in detail the contributions of the geometrical factors including the effects caused by the STM tip curvature, point contacts between the tip and the nanotube, charge spreading along the nanotube during tunneling, and so on with a jellium model potential. Utilizing recent advances in computer power and a new carbon pseudopotential we can incoporate the atomic structure into our model. We investigate wave packet tunneling from the STM tip into the nanotube for n,m indices representing metallic and semiconducting nanotubes. First results of this calculation are presented and compared to ab-initio calculations.

INTRODUCTION

Scanning Tunneling Microscopy (STM) is one of the main techniques to investigate carbon nanostructures [3] and devices fabricated from them. STM images, however, always contain both the effect of the geometry and the electronic structure. As proved by ab-intio calculations [4], essential features of atomic resolution STM images of single wall carbon nanotubes (SWCNTs) can be succesfully and effectively calculated [2,5,6] with the tight-binding method. Some of the features of the STM image, however, are of purely geometrical origin [1]. To investigate these geometrical effects without the effect of the specific atomic structure, formerly we performed wave packet (WP) scattering simulations [7–9] for jellium models of STM tip – CNT – support tunnel junctions. With this simple model, we were able to explain [9] that the STM tip cause apparent broadening [1] of CNTs, and that the displacement of the tunneling point on the surface of the tip during scanning of the CNT causes an apparent asymmetric distortion [5] of the atomic lattice.

Recent advances in computer power make it possible to include the details of the atomic structure into the 3D WP calculations. First results of these atomistic calculations are demonstrated in this paper.

CALCULATION METHOD AND RESULTS

The potential of the CNT was modeled by a local one electron pseudopotential [10] matching the band structure of graphite and graphene sheet. The STM tip and the conductive support surface was modeled by constant potential jellia. The STM tip is taken as a hyperboloid of $0.5\,nm$ apex radius. The CNT is floating above the support plane at a distance of $0.335\,nm$ and the tip – CNT gap is $0.409\,nm$. An armchair $(10,0)$ and a semiconductor $(6,6)$ tube was analyzed. Their diameter is $0.783\,nm$ and $0.814\,nm$, respectively. The tip apex is above an atom in both cases.

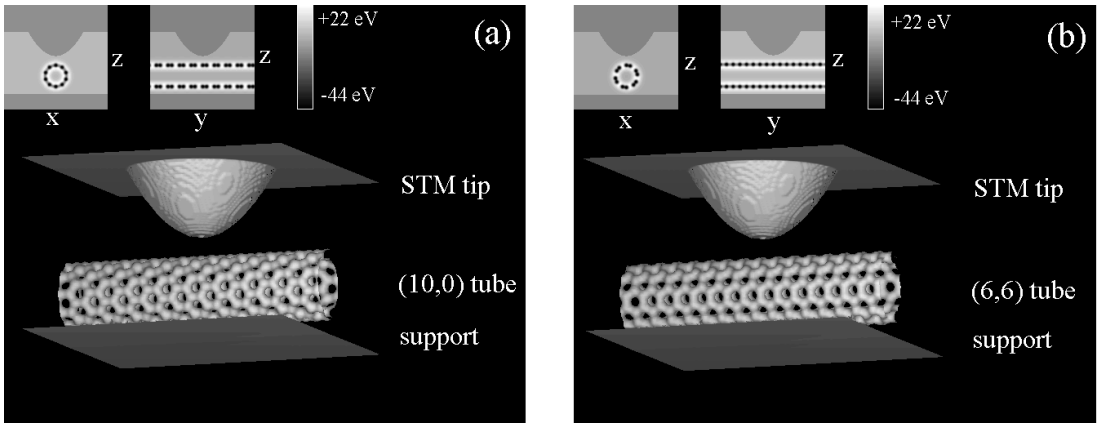

FIGURE 1. One electron local pseudopotential for the STM tip – nanotube – support system. The potential is visualized by the -2.7 eV isosurface. The upper insets show cross sections of the potential perpendicular to the tube and along the tube as grayscale plots. (a) (10,0) tube, (b) (6,6) tube. The apparent fine structure seen on the tip is a gridding artefact.

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 [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 the panel $t = 0.0\,fs$ of *Fig. 2* the initial WP is shown – still in the tip bulk region. The sphere surface is clipped at the upper boundary of the presentation box. At $t = 0.6\,fs$ 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. At $t = 1.8\,fs$ the WP has already tunneled from the tip into the tube

and begins to flow around the tube circumference. The WP flows along the C-C bonds, there is negligible density at the centers of the hexagons because of the large positive value of the pseudopotential there. Note that for the $(6,6)$ tube the WP flows asymmetrically around the tube. This is because the $(6,6)$ tube is not symmetric to the yz plane (the plane containing the axis and the tip apex.) At $t = 3.02\,fs$ the WP already has flown around the tube circumference and begins to spread along the tube. The spreading speed is different for the two tubes.

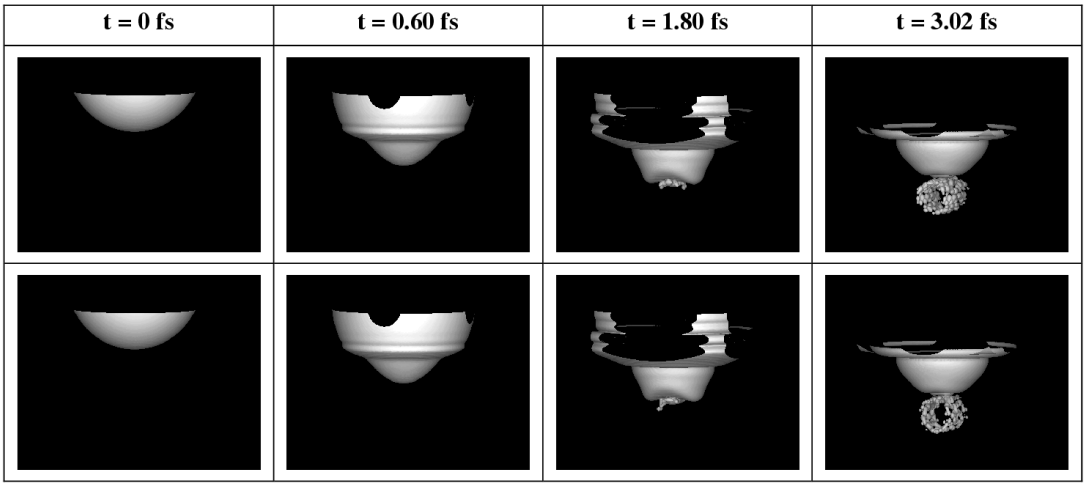

FIGURE 2. Time evolution of the probability density of the wave packet approaching the STM junction from the tip bulk and tunneling into the nanotube. Constant probability density surface is shown. *Upper row*: (10,0) tube, *lower row*: (6,6) tube. The isosurface is clipped at the presentation box boundaries.

DISCUSSION AND CONCLUSION

Fig. 3 shows the isodensity surface of the $(10,0)$ nanotube for $t = 7.25\,fs$. By this time the initial transient has already settled, and the WP is spread over the whole $3.84\,nm$ length of the presentation window. Note that the bonds are charged asymmetrically and the picture is qualitatively similar to that of the ab-initio calculated isosurface seen on *Fig. 1.f.* of Ref. [4]. This is because, as is pointed out in Ref. [4], the wave functions at the Fermi level are a mixture of four different stationary states. The superposition parameters are changing in time.

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. Next we plan to analyze the tunneling of the WP from the tube into the support but this needs somewhat longer simulation time.

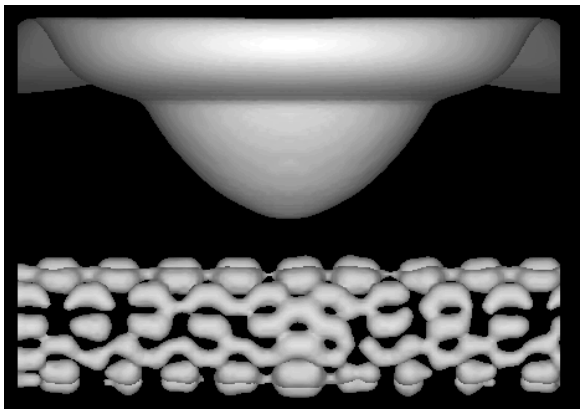

FIGURE 3. Isodensity surface for $t = 7.25\, fs$ viewed from the side of the $(10,0)$ nanotube.

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