Simple Finite Element Model of the Topografiner

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Abstract: We have measured the voltage vs distance $V-d$ characteristics at constant current I of a tunnel junction consisting of an electron emitting sharp tip placed at a variable distance d from a planar anode. At sufficiently large distances, i.e. in the regime of electric field assisted quantum tunneling, the $V-d$ characteristics for different currents follow approximately a power law, the exponent λ being independent of the current. Here we compare and discuss the origin of the observed power law and the measured value of it in terms of electrostatic properties of the tip-plane junction, taking the geometry of the tip as a hyperboloid of revolution.

Keywords: Field-emission electron microscopy.

1. Introduction

A sharp tip approached perpendicular to a conducting surface at subnanometer distances and biased with a small voltage builds a junction across which electrons can be transferred from the tip apex to the nearest surface atom by direct quantum mechanical tunneling. Such a junction is used e.g. in Scanning Tunneling Microscopy (STM). When the distance d between tip and collector is increased beyond some nanometers, the junction enters the electric field assisted regime, the one underlying the topografiner technology –an imaging technique widely used in micro- and nano-electronics. Recent experiments[1] in this regime suggest a scaling law which can be tested numerically by verifying the collapsing of a family of $\Phi(z,d)$-curves, computed at different d, onto one single curve when $\Phi(z)$ is multiplied by a suitable $R(d) \sim d^{\lambda_1}$, see Fig. 1.

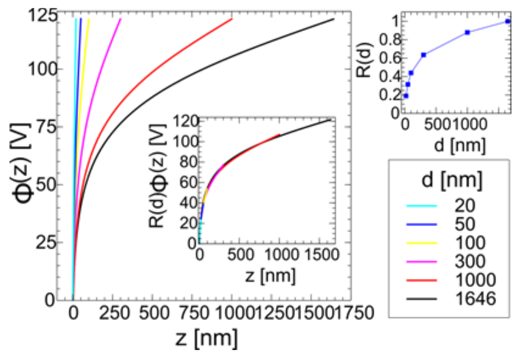

Figure 1. Potential profile $\Phi(z)$ along the tip axis, for a given distance d. The tip used in this COMSOL-simulation is a hyperboloidal model of a "real" tip ($a = 1528$ nm, $\theta_0 = 11°$). The planar counterelectrode is moved between $d = 20$ nm and $d = 1646$ nm. All profiles are made to approximately collapse onto the reference curve by maximal (experimental) value of d when the potential $\Phi(z)$ is multiplied by $R(d)$, this factor plotted in the top corner of the figure, see inset. Notice that both $R(d)$ and the scale profile in the inset behave as a power law[1].

2. The Experiment

Figure 2 shows the scanning tip and the sample in front of this, the setup used for the measurements. For the experiments with the distance d in the sub-nm to nm range the collecting plane (sample) is a W(110) or a Si(111) single-crystal surface, prepared with standard surface techniques in a base pressure of $\approx 10^{-11}$ mbar. By mounting the tip onto a piezocrystal, that can move the tip perpendicular to the surface, the distance can be varied. The value of d was also double checked by means of an optical sensor device, integrated *ad hoc* into our home-made STM microscope.

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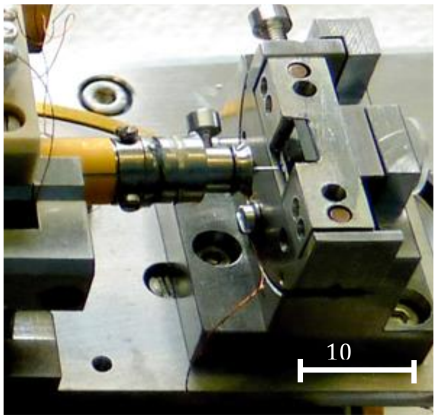

Figure 2. The experimental setup: Tip –and sample-unit of the STM microscope.

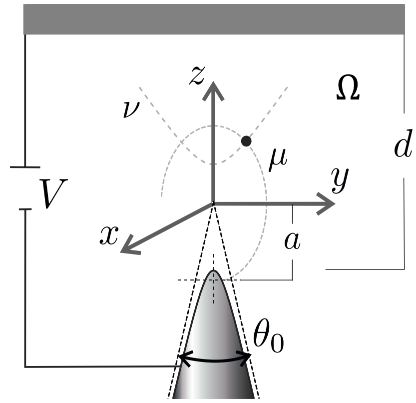

Figure 3. The diodelike tunnel junction modelled within a prolate-spheroidal coordinate system. A point (black dot) in the $z-y$ plane is the intersection between a line of constant prolate spheroidal coordinate μ (an ellipse with focal points at $\pm a$ along the axis z) and a line of constant spheroidal coordinate ν (a hyperbola with focus at $+a$ or $-a$). The hyperboloidal profile has two asymptotic straight lines crossing at the origin of the coordinate system and spanning a full angle of aperture θ_0 which determines the exponent λ in the power law $V \propto d^\lambda$.

3. Governing Equations

A schematic view of the experimental setup is sketched in Figure 3. We consider a conducting tip, defined - within the purpose of this paper - as an infinitely long object with "small" cross section, ending with a more or less sharp apex. A rounding of the cone tip limits its sharpness to nm radius of curvature, depending on the details of the tip preparation in an ultra-high vacuum[2].

3.1 The electrostatic model

In order to consider the electrostatic problem, we have to solve the Laplace equation for the sought for electrostatic potential $\Phi(\vec{\boldsymbol{r}})$ considering the tip and the plane as equipotential boundaries. In addition, we have to consider a "highly symmetric realistic" tip shape. This expression describes the fact that the geometry must be – first – close to the shape one expects for "real" tips (as revealed by a systematic tip imaging via light and electron microscopy[1]) and – second – sufficiently symmetric so that the electrostatic problem can be solved to a large extent analytically. In the used model, the tip, kept at ground potential, is placed vertical to a conducting plane set at the voltage $+V$. The distance between the apex of the tip and the plane is d. Denoting with Ω the region of space excluding the tip and the plane, the electrostatic problem is a well defined Dirichlet problem for the electric potential $\Phi(\vec{\boldsymbol{r}})$:

$$\begin{cases} \nabla^2\Phi & = & 0 & \text{in } \Omega, \\ \Phi & = & 0 & \text{on the surface of the tip,} \\ \Phi & = & +V & \text{on the, plane} \\ |\Phi(x)| & \leq & V & \forall\, \vec{\boldsymbol{r}}(x,y,z) \in \Omega, \end{cases} \quad (1)$$

the last equation being the consequence of the maximum principle of harmonic functions. The solution of this problem is unique and can be computed, at least numerically, in the entire space Ω. However, we will discuss the tunneling current density, which is built up within a very small distance from the tip apex and mainly along the tip axis[3,4]. Accordingly, we focus our attention to finding the behavior of the potential in the vicinity of the tip apex and along the tip axis, i.e. on finding $\Phi(z, x=0, y=0)$ for small z (we set the origin the coordinates $x,\ y,\ z$ at the tip apex). In addition, we will focus on evidencing the scaling behavior of $\Phi(z)$ on the parameters V and d, which are typically imposed experimentally[1].

3.2 The tip as a cone

The cone geometry describes the shape of real tips on the micrometer scale[1]. They contain a true singularity at the tip apex. For both distant ($d \gg 0$) and near (d small) planes the potential has a leading term

$$\Phi(z) \sim V \cdot \left(\frac{z}{d}\right)^{\lambda_1}. \qquad (2)$$

For small angles of aperture of the cone θ_0 (in radians) the exponent λ_1 is given by[5,6] $\lambda_1(\theta_0) \cong [2\ln(2/\theta_0)]^{-1}$. $\theta_0 = \pi$ corresponds to a planar emitter and gives $\lambda_1 = 1$.

3.3 Hyperboloid of revolution

For the tips used in this experiment, not the cone, but the hyperboloid of revolution model is particularly suitable for mimicking the rounded tip with overall conical shape. It has, in fact, two asymptotes that can be used to define a full angle or aperture θ_0. The two asymptotes meet at a point in front of the apex that is located on the so called confocal plane. The focal length a is the distance between this point and the focal point of the hyperboloid, which is located within the tip along the tip axis. For these geometries the scaling properties of the leading potential term depend on whether the plane is "distant" ($d \gg a$) or "near" ($d \ll a$)

$$\begin{cases} \Phi(z) & \sim V \cdot \frac{z}{d} \qquad \text{for} \quad d \ll a, \\ \Phi(z) & \sim V \cdot \left(\frac{a}{d}\right)^{\lambda_1} \cdot \frac{z}{a} \quad \text{for} \quad d \gg a, \end{cases} \qquad (3)$$

with λ_1 being given by same equation as in the cone.

Saint Venant's principle[7] implies an interesting scaling symmetry of the electric field assisted tunneling junction. In fact, one can use this principle to extend the conical solution of the problem[6] to real tips if they can be viewed as a cone with a rounded apex. Because of Saint Venant's principle if the rounding of the cone singularity is local enough – say appears on a length scale a – the conical solution can be used in the following range as well:

$$\Phi(z) \sim V \cdot \left(\frac{z}{d}\right)^{\lambda_1} \quad a \ll z \ll d. \qquad (4)$$

This equation represents a scaling law which can be tested numerically by verifying, e.g., the collapsing of the family of $\Phi(z,d)$-curves, taken for different d, onto one single curve when $\Phi(z)$ is multiplied by a suitable $R(d) \sim d^{\lambda}$.

4. Use of COMSOL Multiphysics

The search for the origin of power laws in this experiment required the systematic study of different electrostatic geometries using the AC/DC COMSOL Module. For the computation of the electric potential, we have fitted a hyperboloid of revolution onto the electron microscope micrograph of the tip used for the taking of the experimental $V-d$-curves. The equipotential surface of the tip was defined with a parametric curve. Subsequently, we have used COMSOL to compute $V(z)$ in the presence of a plane placed at well-defined (large) distance in front of the hyperboloidal tip (Figure 4).

5. Results and discussion

Figure 4 shows an experimental V-d characteristic curve. In a typical experiment, the current is set to some prefixed value. The distance d is then varied and the voltage required to keep the current at the prefixed value is measured. In the range $d \gg 10$ nm, the experimental data follow a power law $\propto d^{\lambda}$, with λ=0.21±0.05. For smaller values of d the dependence becomes

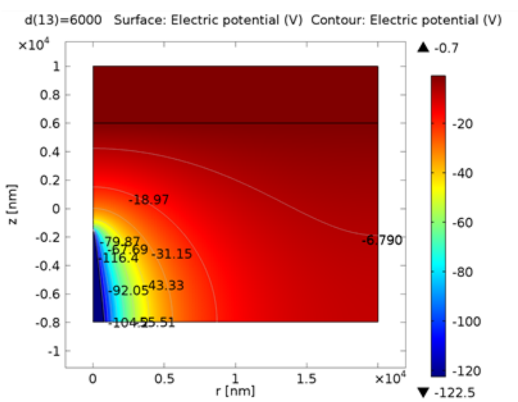

Figure 4. COMSOL-simulation for the diodelike junction showing the electric potential. The tip has a voltage of -122.5 V and the sample in front is set at -0.7 V, as in the experiment.

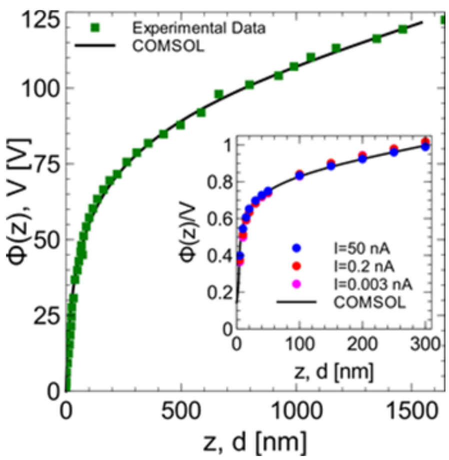

Figure 4. Scaling of $\Phi(z)$ and $V(d)$. The continuos line is the potential profile obtained as described in the caption to Fig., for $d = 1646$ nm. The full squares are $V(d)$ data points obtained at a given current, the current of 150 pA having being chosen so that the $V(d)$ curve almost lies onto the $\Phi(z)$ graph, without need of a rescaling factor. Inset: $V(d)$ data points obtained in a junction with Si(111) at selected currents (given in the inset). The data are rescaled, in the inset, so that they fall onto the same power law. The potential profile computed for $d = 300$ nm (continuos curve) can also be rescaled onto the same curve as the $V(d)$ data.

almost linear, indicating that the junction behaves as a plane capacitor at short distances: Direct tunneling typically occurs in this geometry.

The result of the COMSOL-simulation is also presented in Fig. 4. Notice that a realistic simulation of the full process involving electric field assisted quantum tunneling is a difficult task. It appears, however, on the basis of our simulation, that knowledge of the electrostatics alone is already providing a satisfactory explanation of the observed scaling results. The tip was modeled as a hyperboloid of revolution and the sample was a plane placed at fixed distance $d = 1646$ nm (the largest distance measured in experiment). Plotted in the Figure (blue color) are the values of the electric potential Φ as function of the spatial coordinate x along the tip axis. It turns out that the two curves (COMSOL-simulation $\Phi(x)$ and experiment $V(d)$) can be rescaled onto each other with great accuracy and almost within the entire range. To find an explanation of this similarity –at least on a qualitative level– we turn to the actual process that governs the emission of electron from a sharp tip in the regime of large d: the electric field assisted regime, which can be described by the quantum-mechanical Gamov exponent. In its simplest version, this is given by

$$\frac{\sqrt{8m}}{\hbar}\int_{x_1}^{x_2}\sqrt{\varphi - |e\Phi(x)|}\,dx \qquad (5)$$

φ being the work function of the tip and the spatial integration being performed between the classical turning points x_i. One could agree that the similarity presented in Fig. 4 and the almost power law behavior recorded can be explained by the following Ansatz:

$$\Phi(x) \sim V \cdot \left(\frac{x}{d}\right)^{\lambda}. \qquad (6)$$

This Ansatz would be correct for a conical tip, but both COMSOL-simulation and experiments, which record some deviation from a power law in the small d (and x) regime, suggest that for a realistic tip (with apex rounding) this Ansatz is an oversimplification, although at large distances it works well. We are in the process of finding a more accurate explanation for the similarity between $\Phi(x)$ and $V(d)$ over such large distances. Regarding the value of the exponent λ: our COMSOL-simulations find that the exponent λ is related to the angle of aperture of the hyperboloid, i.e. the angle θ_0 between the axis of
the hyperboloid and its asymptotes. This relation was suggested by Jackson[6] for the analytically solvable problem of a conical tip but it appears to hold true for the more realistic hyperboloidal shape.

A further consequence of Eq. (6) is that an experiment where d is changed and V is adjusted so that the tunneling current (i.e., the potential within the tunneling barrier) is kept constant gives $V \sim d^{\lambda}$, the same power law dependence one expects for the z-dependence of the potential Φ itself. In other words, we expect that all experimental $V - d$ graphs can be made *first* to collapse onto themselves and (see inset of Fig. 4) and *second* can also be collapsed onto a $\Phi(z)$ profile, provided one is not too close to $z = d$ or $z = 0$.

6. Conclusions

In the range $d \gg 10$ nm, the experimental data follow a power law $\propto d^{\lambda}$, with $\lambda = 0.21 \pm 0.05$. For smaller values of d the dependence becomes almost linear, indicating that the junction behaves as a plane capacitor at short distances: Direct tunneling typically occurs in this geometry. These essential features observed experimentally are captured by introducing the potential Φ computed for "realistic" tips into standard equations for electric field assisted tunneling. This highlights the potential of COMSOL-simulation in the context of field-emission electron microscopy.

8. References

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