Simulation of low energy electrons in Scanning Field Emission Microscopy (SFEM)

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Introduction

The Scanning Tunneling Microscope (STM) is the first example of many different types of scanning Probe Microscope (SPM) that are now in use [1]. Predating the STM was a device known as the Topografiner [2] whereby the tip was further from the sample and used in Field Emission (FE) mode. In the experiments carried out at our laboratory, we are also using the STM in FE mode and we call the technique Scanning Field Emission Microscopy (SFEM). IN SFEM, the tip to sample bias is higher (typically 10s of Volts) than that used in STM. This provides the field emitted electrons with sufficient energy to excite secondary electrons from the surface. However, as soon as the secondary electrons (which typically have an energy much less than the primary electron energies from the tip) emerge from the surface, they feel the electric field from the tip and are forced back down on to the surface. Initial simulations showed that all the generated secondary electrons would be forced back on to the surface [3]. Hence one has to ask how is it possible to detect the secondary electrons which are regularly observed in our experiments ?. One solution is that according to quantum mechanics, when a particle experiences a strong accelerating force, it may reflect away from such a force instead of being accelerated in the usual classical manner [4]. This could lead to a reflection of electrons from the surface in SFEM. In addition, simulations of the electrons within the material via a Monte Carlo method would also improve the accuracy of simulations. This has already been carried out by Werner et al. [5], but we wish to double check their simulations as they do not seem to explain all our observations.

The Scanning Field Emission Microscope (SFEM).

The SFEM is essentially the same as an STM, but with the extra provision that the tip can be backed away from the sample and a much higher potential can be applied to the tip. This generates secondary electrons which can be energy analysed and detected using standard (and novel) electron energy analysers [6]. A schematic of the tip region is shown in Figure 1.

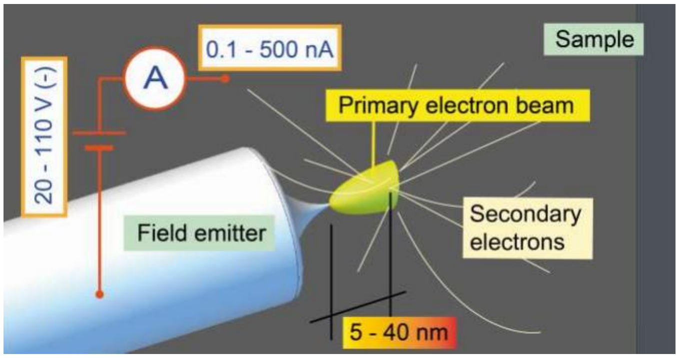

Figure 1. The electrostatic junction in the SFEM.

Simulation of the electrostatic field in the tip-sample region.

A COMSOL model of the SFEM tip-sample region has been previously reported [7] and was used as the basis for the work here.
The COMSOL AC/DC Module was used to solve Laplace equation and calculate the electric potentials and fields. The inputs were Bias-voltage and the distance between tip and sample. This was a stationary study.
The sample was only 400 nm in diameter, in order to limit the computational cost of the simulations, but larger diameter samples are envisaged.
A multislice view of the potential is shown in Figure 2.

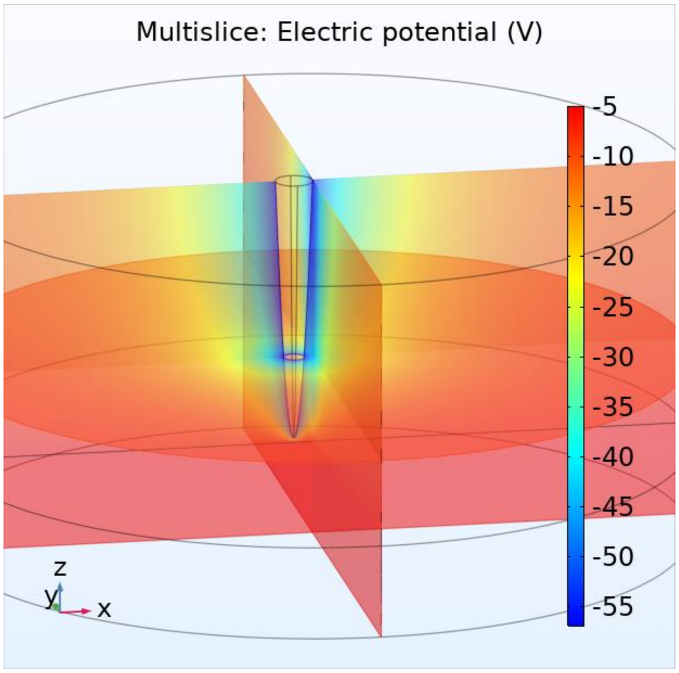

Figure 2. A multislice view of the tip-sample region showing the electrostatic potential.

Since the tip can be just a few nm away from the sample, the electric field in this region can be very strong, but much weaker further away. Ultimately, we need to simulate the electron trajectories up to about 1 mm away from the tip which can have around six orders of magnitude weaker field than at the tip.

For this contribution, however, we will concentrate on the immediate tip-sample region (i.e. 200 nm radius around the tip).

Simulation of the electron trajectories.

For the simulation of the electron trajectories in vacuum, the COMSOL Particle Tracing Module was used. Trajectories were simulated for only a small number of electrons (e.g. 200) by solving the time dependent particle tracing equations. The inputs were the: initial kinetic energy and positions of the secondary electrons. Once the electrons strike the surface, there is a possibility (defined by rules of quantum mechanics) that the electrons can bounce [4]. According to Cazaux [4] the electron reflectivity as a function of the angle of incidence, α, is given by:

$$R(\alpha) = \frac{(1-\sqrt{G})^2}{(1+\sqrt{G})^2}$$

where

$$G = 1 + \frac{E_S - E_k}{E_k cos^2\alpha}$$

where for an insulator (χ= electron affinity)

$$E_S = E_K + \chi$$

and for a metal (E_F = Fermi energy and ϕ is the work function)

$$E_S = E_K + E_F + \phi$$

and E_K is the kinetic energy of the electron.

If the electron is not reflected at the surface, it is assumed to enter the material. In order to simulate electrons in the material, the parameters describing the electron trajectories are handed over to a Monte Carlo program [8]. The electron trajectories in the material are then determined by the elastic and inelastic scattering processes within the material. Should any electrons return to the surface and have sufficient energy to escape back into the vacuum, the parameters describing their trajectory are passed back to COMSOL for further simulation in the vacuum. The above process continues until all electrons have lost sufficient energy that they cannot escape from the material or they have reached the edge of the simulation volume. The whole process is controlled by a shell script.

Results and Discussion

In our simulations, we launch the electrons from the surface rather than the tip. The purpose of doing this is to explore where electrons of a certain energy can escape the tip region and contribute to the signal detected. Figure 3 shows the electron trajectories for 200 electrons with 10 eV launched from the surface directly under the tip. One can see that some of the electrons bounce, but only one escapes from the tip region. However, the simulation shown in Figure 3 does not include the Monte Carlo simulation.

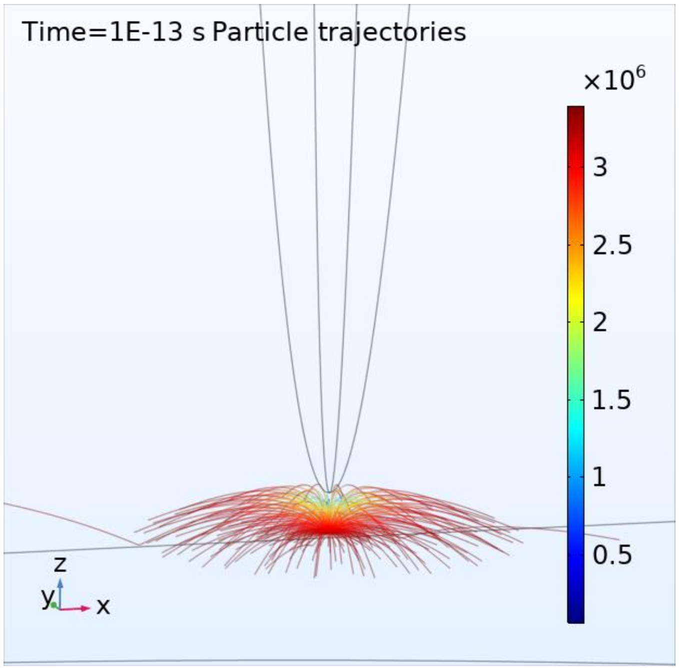

Figure 3. Electron trajectories of 10 eV electrons launched from the surface directly under the tip. The potential between the sample and the tip is 30 V. The colour of the ray is representative of its´s velocity (m/s).

One problem with the approach we are taking is that simulation results require several runs of the COMSOL and Geant4 Monte Carlo program. As such, the output is placed into various files. In order to combine the results into a single image, COMSOL engineers have built an extra facility into the Geometrical Optics module. We hope to take full advantage of this new feature, but there was insufficient time to fully implement it and show the results in this paper.

Conclusions

We have built a model that combines COMSOL particle tracing with an external Monte Carlo model. This approach could be used with a variety of other freely available Monte Carlo programs. The output describing the electron trajectories is placed in several files and needs to be reconstructed using a new feature in the Geometrical Optics module.

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