

Scientific Report: EIPAM Exchange Grant 528

Beneficiary: Dr. Paul Anthony Kendall, Dept. of Physics and Astronomy, Open University, Walton Hall, Milton Keynes, MK7 6AA, United Kingdom

Host: Prof. Jose Ignacio Pascual, Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195, Berlin, Germany

Purpose of the visit

Scanning Tunnelling Microscopy (STM) is a relatively new technique allowing imaging of molecular systems with atomic resolution. The technique relies on the quantum mechanical phenomenon of tunnelling where particles are able to “tunnel” through potential barriers that would classically confine the particles. In an STM electrons tunnel between a ~9 Angstrom radius tungsten tip and a conducting sample (Tersoff 1985). Careful monitoring of the tunnelling current while the STM tip is scanned over the sample allows the tip-sample distance to be measured and a topographical map of the sample to be produced. Hence, with the ability to achieve atomic resolution, an STM offers the unique property of providing an image of the electronic orbitals of the atoms/molecules of the sample surface and any adsorbates lying upon it.

An exciting development of the STM is using the tip to manipulate individual molecules. This can be achieved broadly by two means: 1) Lateral manipulation, 2) Vertical manipulation. Lateral manipulation involves moving the tip close to the surface and making a movement parallel to the surface. The attractive (pulling mode) or repulsive (pushing mode) force between tip and molecule can cause movement or, in some cases, modification of the molecule. Vertical manipulation involves moving the tip close to the molecule and applying a “large” (few Volt) voltage pulse. These manipulations and indeed just scanning the surface with high bias voltages (Sloan 2005) can cause a number of manipulations, e.g. translation, rotation, isomerisation, desorption, dissociation, chemical reactions, etc. The logical conclusion is that if sufficient knowledge of the parameters (bias voltage, tunnel current, location of manipulation, etc.) of individual manipulations can be obtained, a precise tool for molecular scale “surgery” becomes available (e.g. Sloan 2005).

The work intended for this project was twofold. In the first instance it was intended that the STM at Berlin should be used to attempt to develop knowledge relating to the study and manipulation of nucleotide bases (adenine, cytosine, guanine, thymine, uracil) on metal surfaces. This has direct relevance for the interaction of low energy radiation with DNA. In the second instance the knowledge gained from working in Berlin is intended to be transferred to my home institution (Centre of Atomic and Molecular Engineering (cAME) at the Open University). It is intended that a low temperature STM will be installed at cAME around the beginning of 2006 and

that the techniques learned in Berlin will be applied at cAME to continue the studies in this area of radiation damage to biological molecules.

The group of Professor Pascual has a wealth of experience in using STM. The group has access to a homemade low temperature ($\sim 5\text{K}$) STM for 50% of available working time. The time of my visit was advantageous as a new homemade STM was in the final stages of construction and testing during my visit to Berlin. Hence, as well as being able to use a working STM it was possible to observe and participate in the construction of a new machine.

Description of work carried out and results

Most of the time was spent working with the members of the Pascual group. At times when the group had control over the shared STM I was able to observe the experienced users in the group and assist in their investigations. When the group did not have control of the STM I was able to learn to use SPA-LEED apparatus, assist with the construction of the new STM and spend time with another STM group performing molecular switching experiments. The visit allowed me to learn many new techniques:

1) I now have experience of running UHV systems at LHe temperatures. This calls for different techniques to my previous work using HV systems at room temperature and higher operating temperatures (see Kendall (2001) for details of previous research apparatus).

2) In addition to learning STM techniques I have also been able to use other surface science apparatus including SPA-LEED. This is important as it is intended that a LEED unit will be incorporated as an integral part of the planned STM to be installed at the Open University.

3) I have been able to work with AG Pascual to use the low temperature STM to obtain images of various systems of adsorbates/substrates. These include C_{60} Fullerenes + Triptycene on Au (111) and TTF on Au (111). Each combination of adsorbate and substrate requires different imaging conditions and I had the opportunity to experiment with the STM software.

4) Using the STM to manipulate atoms/molecules on the surface was an important goal in the work undertaken. I have been able to learn to use the STM to perform various manipulations using the techniques of vertical and lateral manipulation. This experience included working with another group to “switch” azo-benzole molecules between para and meta configurations.

5) I also learned how to use the STM to perform spectroscopy measurements. These are dI/dV and d^2I/dV^2 spectroscopy where the conductance of the tip-molecule-sample system is measured by varying the bias voltage applied between

the tip-molecule and can be used to deduce position of the molecules electronic orbitals (e.g. HOMO/LUMO) and molecular vibrations.

6) As part of the use of the STM I learned how to prepare samples for measurement. This includes both cleaning samples with sputtering and annealing cycles and dosing the sample with the required adsorbates.

7) I was fortunate to be working with AG Pascual at the point in time when the new low temperature STM was being constructed and tested. This gave me the opportunity to closely inspect the inside of the system including the STM "optics" which are usually contained within radiation shields. Hence, this was a unique opportunity to study the workings of the machine. It also allowed me to get involved with the final pieces of construction and testing. In particular it allowed me to learn new practical skills including the etching of sharp tungsten tips for the STM and using workshop machines to construct metal parts. These skills will continue to be useful in my continuing scientific career.

8) An unfortunate side effect of using delicate UHV apparatus is the tendency for various breakdowns to occur. This, however, allowed me the opportunity to learn about repairing the various apparatus and is as important as learning how to use a fully working STM!

In addition to the various things learned, the visit to Berlin has allowed me the opportunity to progress as a scientist in a number of ways.

1) The FU has many outstanding scientists and I was fortunate to be able to meet and talk with the members of AG Pascual and AG Reider. This allowed me to both increase my scientific knowledge and to network with leaders in the field of STM. This will prove useful in the future work at the Open University.

2) I was fortunate to be given the opportunity to give a seminar about the previous work I had performed at UCL during my PhD (Kendall 2003). This allowed me to develop my presentation skills as well as communicate some of the important results obtained during this work.

3) Having access to both the members of staff at FU Berlin and the excellent seminars given there I have been able to gain knowledge of not only STM but also many other aspects of physics. In the STM field this included both theoretical and practical applications which complimented the lab-based work. In other fields I was fortunate to see seminars by world leading scientists on cosmology, nano-technology and superconductors to name only a few.

4) I have always been interested in learning languages and the visit allowed me to improved my German language skills and experience living in a foreign country for an extended period of time.

The information learned during the visit will be of extreme usefulness in the near future when the cAME group will set up its own STM apparatus. Unfortunately, the fact that the STM was only available for 50% of the total time combined with existing pre-planned work on other adsorbate/substrate systems and a number of problems requiring lengthy repair times (as is the case in UHV systems) meant that the specific work on nucleotide bases was unable to be performed in the time period. However the skills learned in Berlin will allow the experiments to be performed when the cAME STM is installed in the near future.

Future collaboration with host institution

As the groups of Professor Pascual at the Freie Universität and Professor Mason at the Open University are members of the EIPAM network and will, in the future, be involved in similar work it is to be hoped that there will be many opportunities for future collaboration. As a newcomer to the field of STM it is important for cAME to be able to collaborate with such eminent groups as AG Pascual and this visit, as well as future collaborations, will prove invaluable. It is possible in the short term that further visits will be made to Berlin for training purposes and collaborative measurements.

I would like to take the opportunity to thank all involved in this visit to Berlin. Firstly EIPAM for the generous grant that allowed me to take the fantastic opportunity to work at the FU in Berlin. Secondly, thanks to Professor Pascual and his group for allowing me to work with them and for patiently instructing me in the use of a low temperature STM and thirdly to Professor Mason for providing the opportunity of sending me to Berlin.

References

- Kendall, P.A. and Mason, N.J., J ELECTRON SPECTROSC 120 (1-3): p27 OCT 2001
Kendall, P.A., PhD Thesis "Spectroscopic Studies of Atmospheric Molecules Related to Global Warming", University of London, 2003
Sloan, P.A. and Palmer, R.E., NATURE 434, p367: MAR 2005
Tersoff, J. and Hamann, D.R., PHYS REV B 31 (2): p805, JAN 1985