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ELECTRON TUNNELING MICROSCOPY(U) CALIFORNIA INST OF
TECH PASADENA J D BALDESCHWIELER 01 OCT 87

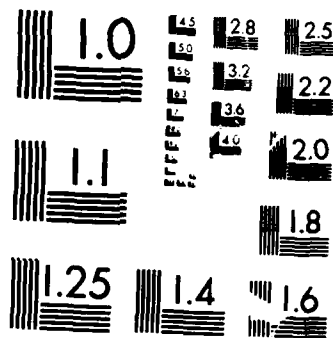
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Dr. John D. Baldeschwieler, Professor of Chemistry

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19. ABSTRACT

The high vacuum STM system at Caltech has been applied to study the surface structure of MoS_2 . The resolution in the plane of the surface is about 1Å, while that normal to the surface is better than 0.1Å. We find that it is straightforward to distinguish two distinct atomic sites at this surface by tunneling microscopy, both in the conventional constant current variable height mode as well as in the variable current constant height mode. The top layer of MoS_2 consists of a hexagonal lattice of sulphur atoms with 3.16Å spacing. Below this plane is an identical lattice of Mo atoms laterally displaced so as to reduce the 6-fold S planar rotational symmetry to three-fold symmetry. The surface unit cell is diamond shaped with four atoms of one type (probably sulfur) at the corners. A single atom of the other type is centered in one triangular half of the cell and a hollow located in the other half. The variation in tunnel current through a series of cell diagonals and cell edges reveals a repeated pattern of three sites along the former and only simple sinusoidal modulation along the latter.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT

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22a. NAME OF RESPONSIBLE INDIVIDUAL

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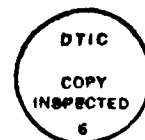
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19. Abstract (continued)

A circular feature about 10A in diameter has also been observed on the MoS₂ surface. This feature can be "easily read" by STM and could perhaps be the basis for encoding information on the surface with a 10A feature size.

We have also carried out an extensive analysis of the structure observed on planar graphite samples under ambient conditions. It is clear that contamination of the tunneling tip with graphite flakes or particulates determines the qualitative appearance of the images which we have obtained.



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ELECTRON TUNNELING MICROSCOPY

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End-of-Year Report

Part I.

- a.1. Michael Weimer, John Kramar, Chunli Bai, and John D. Baldeschwieler "Tunneling Microscopy of 2H-MoS_2 : A Compound Semiconductor Surface" Phys. Rev.B Rapid Communications 1987 submitted. (Shell Companies Foundation)
2. Michael Weimer, John Kramar, Chunli Bai, William J. Kaiser and John D. Baldeschwieler "STM Investigation of 2H-MoS_2 : A Layered Semiconducting transition-Metal Dichalcogenide, Proceedings of 1987 Conference on Scanning Tunneling Microscopy.
- b.1. Richard J. Colton, Shenda M. Baker, John D. Baldeschwieler "An Oxide-free Tip for Scanning Tunneling Microscopy", Appl. Phys. Letts. 1987, 51, 305-307. (Shell Companies Foundation and NIH)
2. Richard J. Colton, Shenda M. Baker, Robert J. Driscoll, William J. Kaiser, Michael G. Youngquist and John D. Baldeschwieler "Imaging Graphite in Air by Scanning Tunneling Microscopy: Role of the Tip" J. Vac. Sci. and Tech A 1987 submitted. (Shell Companies Foundation and NIH)
3. Robert J. Cave, David V. Baxter, William A. Goddard and John D. Baldeschwieler "Theoretical Studies of Electron Transfer in Metal Dimers: $\text{XY} + \text{X} + \text{Y}$, Where $\text{X}, \text{Y} = \text{Be}, \text{Mg}, \text{Ca}, \text{Zn}, \text{Cd}$ " J. Chem. Phys. 1987, 87, 926-935. (Shell Companies Foundation and NIH)
- c.-h. None
- i. Three talks at the Scanning Tunneling Microscopy 1987, Oxnard, California
1. Terry R. Coley, William A. Goddard III and John D. Baldeschwieler "Modeling the STM with *Ab Initio* Theoretical Studies of Electron Transfer in Metal-Metal Cluster Systems".
2. Richard J. Colton, Shenda M. Baker, Robert Driscoll and John D. Baldeschwieler "Imaging Graphite in Air by scanning Tunneling Microscopy: Role of the Tip".
3. Michael Weimer, John Kramar, Chunli Bai and John D. Baldeschwieler "STM Investigation of 2H-MoS_2 : A Layered Semiconducting Transition-Metal Dichalcogenide".
- j. None
- k. Graduate Students: John Kramar, Robert Driscoll, Shenda Baker, Terry Coley, Michael Youngquist
- l. Postdoctoral Fellows: Michael Weimer, Chunli Bai, Richard Colton (Visiting Scientist from the National Research Lab)

Part II.

a. Dr. John D. Baldeschwieler

b. Dr. David Nelson

c. 818-356-6088

d. Brief Description of Project:

Within the past few years a new technique for surface studies has been introduced by Binnig et al.¹⁻⁸ which is capable of atomic resolution. This method, called Scanning Tunneling Microscopy (STM), involves positioning a probe a few angstroms from the surface of interest using a piezoelectric ceramic. A small potential is applied across the gap and the electron tunneling current is measured. The probing tip is then scanned across the surface in two dimensions also using piezoelectric ceramics while adjusting the distance between the tip and surface to maintain a constant current. In this way the tip is made to follow the contours of the surface. The resolution obtained in this way is about $1\text{\AA}$ in the surface plane, and $0.1\text{\AA}$ normal to the surface.

The development of a high-vacuum STM system based on the design pioneered by the IBM Research group in Zurich, and an STM system which operates under ambient conditions based on a design developed by Dr. William Kaiser at the Jet Propulsion Laboratory have been completed by our group at Caltech. Atomic resolution imaging has been demonstrated for both systems.

e. Significant Results During the Past Year:

The high vacuum STM system at Caltech has been applied to study the surface structure of MoS_2 . The resolution in the plane of the surface is about $1\text{\AA}$, while that normal to the surface is better than $0.1\text{\AA}$. We find that it is straightforward to distinguish two distinct atomic sites at this surface by tunneling microscopy, both in the conventional constant current variable height mode as well as in the variable current constant height mode. The top layer of MoS_2 consists of a hexagonal lattice of sulphur atoms with $3.16\text{\AA}$ spacing. Below this plane is an identical lattice of Mo atoms laterally displaced so as to reduce the 6-fold S planar rotational symmetry to three-fold symmetry. The surface unit cell is diamond shaped with four atoms of one type (probably sulfur) at the corners. A single atom of the other type is centered in one triangular half of the cell and a hollow located in the other half. The variation in tunnel current through a series of cell diagonals and cell edges reveals a repeated pattern of three sites along the former and only simple sinusoidal modulation along the latter.

A circular feature about $10\text{\AA}$ in diameter has also been observed on the MoS_2 surface. This feature can be "easily read" by STM and could perhaps be the basis for encoding information on the surface with a $10\text{\AA}$ feature size.

We have also carried out an extensive analysis of the structure observed on planar graphite samples under ambient conditions. It is clear that contamination of the tunneling tip with graphite flakes or particulates

determines the qualitative appearance of the images which we have obtained.

f. **Brief Summary of Plans for Next Year's Work:**

It is proposed to continue the development of the Caltech STM systems with the objectives of studying chemical systems and processes on surfaces. We propose to continue the studies of layered compounds such as MoS_2 with the objective of understanding the role of interstitial defects on surface images, and understanding how to both write and read features on the surface more reproducibly.

Unfortunately, pyrolytic graphite does not appear to be an appropriate substrate for the study of molecular species. We propose to explore the suitability of other substrates such as gold, as well as the chemistry required to bind molecular species covalently to the substrate. We also propose to continue molecular calculations designed to develop a theoretical model for the tunneling of electrons from a probe to a surface with molecular species absorbed, and with atomic and molecular species intervening between the probe and surface.

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