Final Report
DOE-EPSCoR AWARD

Title: Atomistic Studies of Nanotribology
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Major Accomplishments:

DOE-EPSCoR funding for Professor Talat Rahman's research group at Kansas State University has led to an understanding of the microscopic processes that are responsible for manipulation of atoms on metal surfaces. By mapping out the morphology of the potential energy surface seen by an adatom (a solitary atom) in the presence of the tip of a Scanning Tunneling Microscope, Rahman and co-workers have quantified the changes in the activation energy barrier for the diffusion of the adatom in the vicinity of the tip. These results provide good explanation for the experimental observations made in research groups of Professor Rieder at Free University, Berlin, in which a copper atom was found to follow the motion of a STM tip along the edge of a stepped single crystal copper surface, and in Professor Schneider's group in Lausanne, in which a silver atom was found to hop along specific directions on a single crystal silver surface in the presence of a STM tip. These studies also elaborate on structural relaxations brought about by the close vicinity of the tip atoms to those of the substrate. Atomic relaxations are found to be significant for specific tip and substrate atoms and depend on the local coordination (the number of nearest neighbors) at the site of concern: the larger the deviation from bulk-like coordination the larger the relaxation. In general, the trend in the relaxation of the tip and surface atoms can be rationalized on arguments based on local coordination and bonding. Calculations of lateral manipulation of an adatom were carried out on the (111) surface of six metals (Ag, Cu, Au, Ni, Pd, Pt) in which the tip, adatom and the substrate were composed of the same metal. In two other sets of calculations, the tip and the substrate were taken to be made of different materials: Cu tip on Pt(111) and Pt tip on Cu(111), while the adatom was same as the substrate metal. These comparative studies were performed to get insights into the relative ease of lateral manipulation as a function of tip/substrate composition. Manipulation was found to require the least energy on Ag(111). It was also much easier to manipulate a Pt atom on Pt(111) with a Cu(100) tip than the other way around. The variation of the tip shape and geometry also had interesting effects on the manipulation process. In related studies, vertical manipulation of the adatom with a tip was also examined. A comparative study shows that it is easier to manipulate an adatom vertically from a step or a kink site on a surface than from a flat fcc(111) surface. This interesting result can also be

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understood on the basis of tip induced changes in the bonding of the adatom and its low coordinated surroundings.

A significant part of the time of the PI and graduate student Chandana Ghosh was spent in development of two other calculational techniques for future studies. The first of these techniques was the application of *ab initio* electronic structure methods to obtain a more accurate description of the energetics and electronic and geometric structure of the system. This state-of-the art technique is very computer intensive and application to surface systems with defects like steps and kinks (because of reduced symmetry) is non-trivial. The code for such applications is now complete and will be used in future studies, depending on availability of new funds. The second technique drives from the need to examine larger scale systems, than the ones in the above set of studies, and is based on the kinetic Monte Carlo method. Rahman's group has already applied this technique to examine growth patterns and thin film morphology on vicinals of Cu(100). By combining the two techniques, Rahman and co-workers will be able to examine the process of atom manipulation and the nature of atomic scale frictional forces in more detail in the future.

These theoretical and computational studies of the dynamics of adatoms on single crystal surfaces, in the presence of tips, illustrate that atomic manipulation is possible not only when instruments are operating as STM but also in the AFM (Atomic Force Microscope) mode. With the development of codes for *ab initio* electronic structure calculations Rahman and coworkers are finally in a position to carry out studies in tandem with experiments in Dr. Salmeron's group at Lawrence Berkeley Laboratories in which Ag adatoms and small clusters will be manipulated on Pd surfaces. The objective of these studies is to understand the types of interactions that exist between atoms in regions of low coordination, to get insights into the nature of the atomic bonding which would eventually facilitate the control and manipulation of important chemical reactions and the nanostructuring of materials. The work involving AFM studies is expected to provide insights into atomic-scale frictional forces measured by Dr. Salmeron's group on passivated Pd and Pt surfaces.

Publications To Date:

1. U. Kuerpick and T.S. Rahman, Tip Induced Motion of Adatoms on Metal Surfaces," Phys. Rev. Lett. 83, 2765 (1999).
2. T. S. Rahman, "Simulations of Surface Phenomena," in Methods in Materials Research, Ed. J. M. Sanchez, J. Wiley, NY (2001).
3. C. Ghosh, A. Kara, and T.S. Rahman, "Theoretical aspects of vertical and lateral manipulation of atoms," Surf. Sci. **502/503**, 519 (2002).
4. M. Rusanen, I. T. Koponen, T. Ala-Nissila, C. Ghosh, and T. S. Rahman, "Morphology of ledge patterns during step flow growth of metal surfaces vicinal to fcc(001)," Phys. Rev. B **65** (Rapid Comm.), 041404 (2002).
5. C. Ghosh, A. Kara and T. S. Rahman, "Adatom Manipulation and Tip Induced Relaxation of Atoms," submitted to Phys. Rev. B.
6. R. Heid, A. Kara, K. P. Bohnen, and T. S. Rahman," *Ab initio* Calculations of Multilayer Relaxations of Stepped Cu Surfaces," Phys. Rev. B. **65,** 115405 (2002).

Talks and Presentations: A total of 3 invited talks and 6 contributed talks were presented on the above topic by Rahman and Ghosh.

Award or Honor to Personnel:

Award: Distinguished Graduate Faculty Award, 1998
Recipient: Professor Talat S. Rahman
Issued by: Commerce Bank / Kansas State University

Award: Fellow of the American Physical Society, 1998
Recipient: Professor Talat S. Rahman
Issued by: American Physical Society

Award: Alexander von Humboldt Research Prize, 2000
Recipient: Professor Talat S. Rahman
Issued by: Government of Germany

Award: University Distinguished Professor, 2001
Recipient: Professor Talat S. Rahman
Issued by: Kansas State University

Award: Best Poster Presentation by a Graduate Student
Recipient: Chandana Ghosh (PhD Supervisor: Dr. Talat S. Rahman)
Issued by: Organizing committee, Ninth International Workshop on Surface Dynamics, Virginia, June 2-6, 1999
Poster Title: "Tip Induced Shift of the Diffusion Saddle Point"

Development of Human Resources:

Graduate student Chandana Ghosh was supported for three years on this grant. She is finishing the requirements of her PhD degree and is expected to complete them by May 2003. Some funds were also provided to Dr. A. Kara, who has now become an expert on electronic structure calculations, in addition to his previous expertise.