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13. ABSTRACT *(Maximum 200 words)*

The research program focused on formulation, development, implementation and application of novel modeling and large-scale atomistic classical and quantum molecular dynamics simulations, for investigations of critical issues in areas of basic and technological importance. These studies include: atomic-scale processes and mechanisms underlying tribological phenomena and thin-film lubrication; mechanical, electronic and transport properties of nanoscale interfacial junctions; structure and thermodynamics of nanocrystalline systems and surface diffusion of adsorbed nanoclusters. Research achievements include: (1) Development of a grand-canonical molecular dynamics simulation method allowing large-scale studies of structure, dynamics, rheology and lubrication mechnisms in narrow junctions; (2) Comparative simulations of model lubricants charaterized by different molecular shapes, sizes and structural complexity, resulting in ellucidation of the energetic and entropic origins of layering transitions and solvation force oscillations in lubricated junctions under high loads; (3) Discovery of a novel method for controlling and reducing friction, as well as suppresion of stick-slip behaviour in lubricated junctions, achieved through application of small amplitude oscillations to the sliding surfaces normal to the shear plane; (4) Simulations and discovery of enhanced surface diffusion of large clusters, e.g. gold nanocrystallites with over one hundred atoms adsorbed on graphite, occuring through a collective slip-diffusion mechanism.

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<u>Final Report</u>

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Microscopic Modeling of Nanotribology, Elastohydrodynamics, Lubrication and Interfacial Systems

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Period: August 1, 1996 - July 31, 1999

1. Objectives

The focus of the research program supported by this grant is the formulation, development, implementation and application of modeling strategies and large-scale computer simulation methods for studies of critical issues in three main areas:

(i) Tribological Interactions, Nanomechanics, Thin Film Lubrication, and dynamical and rheological properties of thin films of complex molecular liquids.

(ii) Mchanical and electric properties of interfacial junctions; nanowires.

(iii) Nanocrystals and their two and three-dimensional assemblies; geometrical and electronic structures, thermodynamics and dynamics.

The program serves as a focus for investigations in materials science and computational methodologies regionally, nationally and internationally. Several of our projects are performed in collaboration with experimental laboratories (e.g. investigations of nanocluster assemblies and conductance in nanowires at Georgia Tech, and studies of friction control at the University of California, Santa Barbara). In addition to the scientific goals the program fulfills educational ones through the training of post-doctoral fellows, and graduate students (currently one Ph.D. thesis student at GA Tech).

During the current report period the main research efforts were aimed toward the above objectives, coinciding with the objectives listed in the Research Proposal underlying this program.

2. Status and Achievements

Significant progress has been achieved in all of the above main areas of research. In addition a graduate student (Eric Ringer) received his Ph.D. degree (Spring 1999); thesis title:

"The Energetics, Dynamics and Transport Properties of CaF_2: Surface Superionic Conductivity". The main achievements include:

(i) Simulations of Nanotribological Processes

Investigations have been performed focusing on the atomic-scale structure, energetics, dynamics and rheology of model lubricant molecular films confined in narrow junctions by atomically-structured solid interfaces and aiming at providing insights into the behavior of boundary lubricants under high normal load and during shear. This research was enabled by the formulation and implementation of a novel grand-canonical molecular dynamics simulation method.

Major efforts were devoted to the development, implementation and applications of a novel simulation method, which allows systematic investigations of energetics, structure dynamics and rheology of thin film lubricants. The new method (described in two publications by J. Gao, W. D. Luedtke, and Uzi Landman, in J. Chem. Phys. 106, 4309 (1997), and J. Phys. Chem. 101, 4013 (1997)) allows for grand-canonical molecular dynamics (GCMD) simulations of thin films confined by solid substrates. The method combines constant pressure simulations with a computational cell containing solid surfaces and both bulk and confined liquid regions in equilibrium with each other. This configuration allows direct simulations of experiments (such as surface force apparatus (SFA), and tip-based methods (i.e., atomic force and friction force microscopies)), aimed at gaining deep insights into the influence of the molecular structure and the interactions between molecular fluids and the confining solid surface, on the lubrication characteristics under extreme conditions of high loads and shear rates.

Comparative simulations of model lubricants characterized by differing molecular shape, size, and complexity (i.e., globular molecules, straight-chain alkanes of different length such as hexadecane and tetracosane, and a branched alkane, i.e., squalane), revealed the energetic and entropic origins of density layering in such confined molecular liquids and the consequent characteristic solvation forces as a function of the junction width. It was found that while both globular molecules, straight chain alkanes and branched ones exhibit density layering, all but the branched lubricant are characterized by oscillatory solvation forces with a period of the molecular width. The branched alkane which is of higher viscosity in the bulk was found to maintain a higher degree of fluidity under extreme confinement conditions, while the globular and straight-chain molecular liquids tend to undergo under high confinement a transition into a soft solid state, which under shear exhibits solid-like stress accumulation and yield processes leading to molecular scale stick-slip behavior.

We have also shown, using the GCMD method that the rheological properties of a confined lubricant film depend on interfacial commensurability, with commensurate films exhibiting abrupt transitions into a "soft solid" state for relatively thick, 5 or 6 later, films (Phys. Rev. Lett. 74, 705 (1997).

Motivated by our aforementioned findings we have performed extensive comparative GCMD simulations which led us to the discovery of a novel method for controlling and reducing friction in lubricated junctions. In these simulations two surfaces (gold) were brought to a close proximity and the gap between them was filled by a lubricant (the whole system is immersed in a cell containing the lubricant), under a prescribed load. Sliding the two surfaces with respect to each other, under constant load, at a velocity of 1 m/s resulted in stick-slip motion, and a transition to steady-sliding occurred only upon a 20 fold increase in the sliding velocity. However when the surfaces were set again in motion with respect to each other at a velocity of 1 m/s but with an (externally) imposed small amplitude (~ 1 Å) oscillation of the distance between them (that is, perpendicular to the shear plane), the stick-slip dynamics was eliminated and steady sliding occurred accompanied by a dramatic (over ten fold) reduction of the frictional resistance. Through detailed analysis, involving special visualization techniques and a generalized rate-and-state model, we have found that underlying the above phenomena are oscillation induced frustrations of the ordering processes in the lubricant, which through a controlled choice of the oscillation frequency is maintained in a dynamic non-equilibrium state throughout the sliding process.

The findings of this study were reported in a cover article in the Journal of Physical Chemistry B102, 5033 (1998), and it had been highlighted in the July 25, 1998 issue of Science News (154, 61 (1998)). Moreover in an adjacent article laboratory experiments performed by Professor Jacob N. Israelachvili and his colleagues at UC Santa Barbara, verified the theoretical predictions by observing a ten fold decrease upon a 1 Å oscillation in surface force apparatus (SFA) measurements. We believe that this novel method for friction control may find uses in many different situations (such as motors, machines and micro-devices), and it may be generalized also to reduction of frictional energy losses in powders and granular materials during transportation and materials processing.

In addition to the above we have devoted during this reporting period a significant amount of time to parallelization of our friction and lubrication molecular dynamics codes. As a result we are capable now to simulate systems of up to one million particles, which will allow us to explore frictional and lubrication processes in extended junctions and for lubricants of high complexity (including lubricant mixtures and effects due to patterning of the solid surfaces).

(ii) Interfacial Junctions; Nanowires

Understanding the variation of a material's properties with size, form of aggregation and dimensionality is becoming important in the face of increasing miniaturization of electronic and mechanical devices. Experimental studies have focused on the preparation and characterization of solid-state nanometre-scale structures such as metal and semiconductor nanocrystals, surface-supported structures and quantum dots and nanoscale junctions or wires.

(a) It has emerged that these nanostructures can often be fruitfully described using concepts and methodologies developed in the contexts of gas-phase atomic clusters and atomic nuclei. We made this connection explicitly through first-principle molecular dynamics simulations which showed that, as nanowires of sodium metal are stretched to just a few atoms in diameter, the structures formed by metal atoms in the neck can be described in terms of those observed in small gas-phase sodium clusters. We found that the electronic spectral and conductance characteristics of these atomic-scale contacts exhibit dynamical thermal fluctuations on a sub-picosecond timescale, owing to rearrangements of the metal atoms, which will significantly affect the transport properties of such nanowires. (R. N. Barnett and U. Landman, Nature 387, 788-791 (1997)).

(b) In two other publications we investigated thermopower of quantum nanowires in a magnetic field, showing: (1) the occurrence of magnetic field splitting of thermopower peaks associated with electronic energy levels which are degenerate at zero field, as well as proposing a scheme for measuring thermopower in a circuit containing a nanowire and leads made from the same material (Phys. Rev. B 56, 1065-1068 (1996)), and (2) we have investigated the effects of the shapes of the cross sections of three-dimensional nanowires on electronic conductance quantization, and have elucidated the behavior of such wires for both hard- and soft-wall confining potentials (Phys. Rev. B 56, 1065-1068 (1997)).

(c) Energetics and quantized conductance in jellium-modeled nanowires were investigated using the local-density-functional-based shell correction method, extending our previous study of uniform-in-shape wires [C. Yannouleas and U. Landman, J. Phys. Chem. B 101, 5780 (1997)] to wires containing a variable-shaped constricted region [Phys. Rev. B 57, 4872 (1998)]. The energetics of the wire (sodium) as a function of the length of the volume-conserving, adiabatically shaped constriction, or equivalently its minimum width, leads to the formation of self-selecting magic wire configurations, i.e., a discrete configurational sequence of enhanced stability, originating from quantization of the electronic spectrum, namely, formation of transverse subbands due to the reduced lateral dimensions of the wire. These subbands are the analogs of shells in finite-size, zero-dimensional fermionic systems, such as metal clusters, atomic nuclei, and ^{3}He clusters, where magic numbers are known to occur. These variations in the energy results in oscillations in the force required to elongate the wire and were found to directly correlate with the stepwise variations of the conductance of the nanowire in units of $2e^2/h$. The oscillatory patterns in the energetics and forces, and the correlated stepwise variation in the conductance, were shown, numerically and through a semiclassical analysis, to be dominated by the quantized spectrum of the transverse states at the most narrow part of the constriction in the wire.

(d) The excitation energies between electronic modes in metallic (and semimetallic) nanowires are in the microwave range. Consequently, photoconductance and magneto-optic effects can be used for investigations of such wires, as well as providing opportunities for the development of miniaturized sensors in the above frequency range. We investigated effects of irradiation on the electronic conductance in nanowires, for field-free conditions and under the influence of applied longitudinal magnetic fields. The nanowires were modeled within the free-electron framework with a parabolic (transverse) confining potential. Our results for the dependence of the photoconductance of irradiated nanowires on the photon energy and/or the strength of the applied magnetic field show that such measurements may be used as a magneto-optic spectroscopy for determination of (i) the electron Fermi energy, (ii) the electron effective mass, and (iii) the number of quantized modes in the nanowire. Such measurements may also be used to assess to what degree the electron transport through the nanowire is adiabatic. Furthermore, our results suggest a method for controlling and tuning electronic transport in nanowires via external electromagnetic fields [Phys. Rev. B 58, 6064 (1998)].

(e) A theoretical analysis of thermal transport in nanowires, in field-free conditions and under influence of applied magnetic fields, was presented. It was shown that in the nonlinear regime (finite applied voltage) new peaks in the Peltier coefficient appear leading to violation of Onsager's relation between the Peltier and thermopower coefficients. Oscillations of the Peltier coefficient in a magnetic field were demonstrated. The thermo-conductance has a step-like quantized structure similar to the electroconductance and exhibits deviations from the Wiedemann-Franz law. The strong dependence of the thermoconductance on the applied magnetic field, leads to the possibility of magnetic blockade of thermal transport in wires with a small number of conducting channels. Possible control of thermal transport in nanowires through external parameters, that is applied finite voltages and magnetic fields, were discussed. [Solid

State Communications 108, 851 (1998), and Phys. Rev. B 60, (1999), accepted].

(iii) Nanocrystals, Clusters, and Quantum Dots

A. Nanocrystals

Our work in this area was motivated by the size-dependent specificity and selectivity of the physical and chemical characteristics of materials, opening avenues for their use in sensor and electronic technologies. In the following we highlight our main achievements.

(a) In a joint theoretical-experimental study (Phys. Rev. Lett. 79, 1873-1876 (1997)), we addressed the often expected (and observed) behavior that the structures of finite-size materials aggregates differ from those of the bulk. Specifically we have shown that for gold the 1 nm $\leq d_{eq} \leq$ 2 nm size range (where d_{eq} is the equivalent nanocrystallite diameter), is punctuated by the formation of a discrete sequence of primarily three cluster sizes which correspond well to the most stable ones in this range, all belonging to the truncated (Marks)-decahedral motif with the particular truncations described above. This analysis provides an energetic and structural explanation for the observed preferential formation of this discrete sequence of stable gold nanocrystallites in this range. While similar structures of larger metal particles have been discussed experimentally and theoretically, they have not been previously associated with a stable metal cluster sequence in this size range.

Along with a resolution of the structural issue, we demonstrated the ability to obtain macroscopic quantities of highly size-separated nanometer-scale metal clusters in a refined state (i.e., neutral cores with "weak" passivation which does not seem to disrupt the metal nanocrystallite structure). These findings have broad implications for measurements of various size and structure sensitive physical properties (e.g., electronic quantized transport processes in individual particles and their superlattices, and spectroscopic characteristics which are the subject of current research efforts, with a potential application in optoelectronics, nanocircuits, and sensor technologies.

(b) Investigations of the thermal evolution of structural and dynamic properties of gold nanocrystalline clusters of variable size (Au_{75}, Au_{146} and Au_{459}) were performed using extensive molecular dynamics simulations employing embedded atom interactions. These studies revealed that the thermal evolution of these clusters is punctuated by diffusionless solid-to-solid structural transformations from the low-temperature optimal structures (truncated-decahedra for Au_{75} and Au_{146}, and a face-centered-cubic structure with a truncated-octahedral morphology for Au_{459}) to icosahedral structures. These structural transformations are precursors to the melting transitions which occur at temperatures below the bulk melting temperature of crystalline gold, and they are intrinsic to the thermodynamics of the clusters. The melting scenario revealed by the simulations for these gold clusters differs from that involving thickening of a quasi-liquid wetting surface layer, and in addition it does not involve at any stage of the thermal process dynamic coexistence where the cluster fluctuates between being entirely solid or liquid. For the larger cluster, Au_{459}, a thermodynamic (icosahedral) solid-liquid coexistence state was found in the vicinity of the melting transition. The occurrence of polymorphic solid structures, that is a cluster containing simultaneously decahedral and icosahedral parts, was discussed in light of early observations of such structures via high resolution electron microscopy. [Phys. Rev. Lett. 81, 2036 (1998), and Phys. Rev. B 60, 506 (1999)].

(c) The preparation of nanocrystalline materials often requires passivation of the individual particles to protect against modifications of their properties by their environment, as well as to inhibit their propensity to sinter. One of the most elegant passivation routes is through self-assembly, that is spontaneous formation of passivating monolayers of organic molecules (such as n-alkylthiols), which have been shown to provide a viable means of controlling the physical and chemical properties of extended surfaces and nanocrystalline facets.

While formation and properties of self-assembled monolayers (SAMS, particularly n-alkylthiols on gold) on extended surfaces had been studied rather intensively, much less is known about the adsorption, intermolecular organization and thermodynamics of such molecules on finite crystallines (which expose various crystalline facets, edges and corner sites).

In our studies equilibrium structures and thermodynamic properties of dodecanethiol self-assembled monolayers on small (Au_{140}) and larger (Au_{1289}) gold nanocrystallites were investigated with the use of molecular dynamics simulations. We find that compact passivating monolayers are formed on the (111) and (100) facets of the nanocrystallites, with absorption site geometries differing from those found on extended flat Au(111) and Au(100) surfaces, as well as with higher packing densities. At lower temperatures the passivating molecules organize into preferentially oriented molecular bundles with the molecules in the bundles aligned approximately parallel to each other. Thermal disordering starts at $T \geq 200$ K, initiating at the boundaries of the bundles and involving generation of intramolecular conformational (gauche) defects which occur first at bonds near the chains' outer terminus and propagate inward toward the underlying gold nanocrystalline surface as the temperature is increased. The disordering processes culminates in melting of the molecular bundles, resulting in a uniform orientational distribution of the molecules around the gold nanocrystallites. From the inflection points in the calculated caloric curves, melting temperatures were determined as 280 and 294 K for the monolayers adsorbed on the smaller and larger gold nanocrystallites, respectively. These temperatures are significantly lower than the melting temperature estimated for a self-assembled monolayer of dodecanethiol adsorbed on an extended Au(111) surface. The theoretically predicted mechanisms and melting scenario, resulting in a temperature-broadened transition, support recent experimental investigations [J. Phys. Chem. B 102, 6566 (1998)].

(d) Energetics, electronic structure, charging, and capacitive properties of bare and thiol-passivated Au_{38} gold nanocrystals were investigated via density-functional calculations. In the energy-optimized passivated nanocrystal, comprised of a truncated-octahedral face-centered-cubic Au_{38} core coated by a monolayer of 24 methylthiol (SCH_3) molecules, we found interfacial charge transfer of about 2e from the outermost gold atoms to the sulfur atoms. The estimated effective capacitance is 0.084 aF, correlating well with recent electrochemical measurements. Charging takes place within the molecular layer. Molecular adsorption of dimethyl-disulfide was found to be energetically unfavorable for a gold cluster of this size. [Phys. Rev. Lett. 82, 3364 (1999)].

(e) Diffusion processes of atoms, molecules, and clusters on solid surfaces continue to be a subject of active research of basic and technological interest (e.g., in the areas of film growth and catalysis), and a source of discovery pertaining to diffusional energetics and mechanisms. We reported here on a novel surface diffusion phenomenon, where large (hundreds of atoms) three-dimensional gold clusters adsorbed on a graphite surface are predicted via atomistic MD simulations to undergo anomalous diffusive motion with surprisingly high rates, occurring through a collective slip-diffusion mechanism, involving long sliding trajectories, which may be described mathematically as Lévy flights. [Phys. Rev. Lett. 82, 3835 (1999)].

B. Clusters

To understand the nature of interactions of metals and H_2O with semiconductors and ceramics, investigations were performed on the energetics and structure of sodium doped silicon clusters (S. Wei, R. N. Barnett, and U. Landman, Phys. Rev. B 55, 7935 (1997) and of water interaction with small neutral and charged silicon clusters (S. Wei and U. Landman, J. Phys. Chem. A 101, 5035 (1997)).

In the first study energetics and structures of neutral and charged Si_n ($n \leq 10$) and sodium-doped Si_nNa clusters have been investigated using local spin density functional electronic structure calculations and structural optimizations, with and without exchange-correlation gradient corrections. For the Si_n clusters, the monomer separation energies show local maxima for $n = 4$, 7, and 10. The vertical and adiabatic ionization potentials are smaller than the values for the Si atom and exhibit odd-even oscillations with values in agreement with experiments, and the adiabatic electron affinities show local minima for $n = 4$, 7, and 10, with the value for the heptamer being the smallest, in agreement with the experimentally measured pattern. Binding of Na to Si_n is characterized by charge transfer from the sodium resulting in the development of significant dipole moments for the Si_nNa clusters. The binding energy of Na to Si_n oscillates as a function of n, with local minima for $n = 2$, 5, and 9, and local minima for $n = 4$, 7, and 10, with the value for $n = 7$ being the smallest. A similar trend is found for the vertical and adiabatic ionization potentials of the doped clusters, correlating with the electron affinity trend exhibited by the Si_n clusters, and in agreement with recent measurements. In the optimal adsorption geometry of H_2O on the Si_7Na cluster, the oxygen is bonded to the Na, with a hydration energy significantly higher than that of an isolated sodium atom. The vertical and adiabatic ionization potentials of NaH_2O

are lower than those of Si_7NaH_2O, and the values for the latter are lower, by ≈ 0.2 eV, than those of the unhydrated Si_7Na cluster.

In the second study we have shown that water binds to a Si atom in a triplet state, while it does not bind stably to Si_2, forming a Si-Si-H_2 metastable complex in the singlet state. Binding to a larger cluster (Si_7) was found to be very weak. In all cases binding occurs through formation of a Si-O bond, with a partial donation of charge from the oxygen, accompanied by the development of a large dipole moment. These results have implication to the area of porous silicon, and further studies are in progress.

C. Quantum Dots

Measurements on quantum dots (QD's) created in semiconductor heterostructures, containing a (small) adjustable number of electrons (controlled by gate voltages), revealed a remarkable similarity between their spectra (e.g., shell structure) and that of naturally occurring zero-dimensional fermionic systems (e.g., atoms and nuclei) suggesting the naming of these solid-state structures as “artificial atoms”, with potential utilization in electronics and computer technologies. Most recently several investigations have been made toward extending such an analogy to “artificial quantum dot molecules” (QDM's) and “artificial crystals” comprised of coupled quantum dots.

Using a single-particle semi-analytical model and self-consistent electronic structure calculations employing the local spin-density-functional (LSD) theory, we explored the spectra of artificial lateral QDM's with and without external magnetic fields. We illustrated analogies between QDM's and their natural counterparts, and explored the transition from the weakly-coupled dots (tunnel-split) regime to the covalent (delocalized) bonding one as a function of interdot distance, coupling strength, relative well-depth of the coupled QD's (i.e., hetero-QDM's), and magnetic field strength.

In this study we constructed a molecular orbital classification of the QDM states which correlates between the united-dot and separated-dots limits. LSD addition energies and spin polarization patterns for QDM's in the entire coupling range were analyzed, guiding the construction of a constant interaction model. A magnetic field induces decoupling (effective "delocalization" of the QDM) and convergence into a Landau spectrum for strong fields were found. [U. Landman, et al., Europ. J. Phys. D, Vol. 9 (1999), in press].

3. Publications

1. "Thermopower of Quantum Nanowires in a Magnetic Field", E. N. Bogachek, A. G. Scherbakov, and U. Landman, Phys. Rev. B 54, R11094 (1996).
2. "Structural Evolution of Larger Gold Clusters", C. L. Cleveland, U. Landman, M. Shafigullin, P. W. Stephens, and R. L. Whetten, Z. Phys. D 40, 503 (1997).
3. "Nanowires: Size Evolution, Reversibility, and One-Atom Contacts", U. Landman, R. N. Barnett, and W. D. Luedtke, Z. Phys. D 40, 282 (1997).
4. "Energetics and Structures of Neutral and Charged Si_n ($n \leq 10$) and Sodium Doped Si_nNa Clusters", S. Wei, R. N. Barnett, and U. Landman, Phys. Rev. B 55, 7935 (1997).\
5. "Structure and Solvation Forces in Confined Films: A Comparative Study of Straight and Branched Alkanes", J. Gao, W. D. Luedtke, and U. Landman, J. Chem. Phys. 106, 4309 (1997).
6. "On the Origins of Solvation Forces in Confined Films", J. Gao, W. D. Luedtke, and U. Landman, J. Phys. Chem. 101, 4013 (1997).

7. “Cluster-Derived Structures and Fluctuations in Nanowires”, R. N. Barnett and U. Landman, Nature 387, 788 (1997).

8. “Shape Effects on Conductance Quantization in Three-Dimensional Nanowires: Hard versus Soft Potentials”, E. N. Bogachek, A. G. Scherbakov, and U. Landman, Phys. Rev. B 56, 1065 (1997).

9. “Structure and Binding of Neutral and Charged Si_nH_2O (n = 1,2,7) Clusters”, S. Wei and U. Landman, J. Phys. Chem. 101, 5035 (1997).

10. “Layering Transitions and Dynamics of Confined Liquid Films”, J. Gao, W. D. Luedtke, and U. Landman, Phys. Rev. Lett. 79, 705 (1997).

11. “Structural Evolution of Smaller Gold Nanocrystals: The Truncated Decahedral Motif”, C. L. Cleveland, U. Landman, T. G. Schaaff, M. N. Shafigullin, P. W. Stephens, and R. L. Whetten, Phys. Rev. Lett. 79, 1873 (1997).

12. “Friction Control in Thin-Film Lubrication”, by J. Gao, W. D. Luedtke, and U. Landman, J. Phys. Chem. B 102, 5033 (1998).

13. “Energetics, Forces, and Quantized Conductance in Jellium-Modeled Metallic Nanowires”, by C. Yannouleas, E. N. Bogachek, and U. Landman, Phys. Rev. B 57, 4872 (1998).

14. “On Nanotribological Interactions: Hard and Soft Interfacial Junctions”, by U. Landman, Solid State Communications (Special Issue on Frontiers in Condensed Matter Science) 107, 693 (1998).

15. “Structure and Thermodynamics of Self-Assembled Monolayers on Gold Nanocrystals”, by W. D. Luedtke and U. Landman, J. Phys. Chem. B 102, 6566 (1998).

16. “Nanoscale Lubrication and Friction Control”, by J. Gao, W. D. Luedtke, and U. Landman, in “Nonequilibrium Dynamic Processes at Colloidal Interfaces”, edited by Y. Shnidman, (ACS Publications, 1998).

17. “Magneto-Optics of Electronic Transport in Nanowires”, A. G. Scherbakov, E. N. Bogachek, U. Landman, R. Shekter, M. Jonson, I. Gorelik, and S. Blom, Phys. Rev. B 58, 15305 (1998).

18. “Nonlinear Peltier Effect in Quantum Point Contacts”, E. N. Bogachek, A. G. Scherbakov, and U. Landman, Solid State Communications 108, 851 (1998).

19. “Electronic Structure of Passivated $Au_{38} (SCH_3)_{24}$ Nanocrystal”, H. Hakkinen, R. N. Barnett, and U. Landman, Phys. Rev. Lett. 82, 3264 (1999).

20. “Slip Diffusion and Levy Flights of an Adsorbed Nanocluster”, W. D. Luedtke and U. Landman, Phys. Rev. Lett. 82, 3835 (1999) .

21. “Structures and Spectra of Gold Nanoclusters and Quantum Dot Molecules”, R. N. Barnett, C. L. Cleveland, H. Hakkinen, W. D. Luedtke, C. Yannouleas, and U. Landman, Euro. J. of Phys., Vol. 9 (1999), in press.

22. “Nonlinear Peltier Effect and Thermoconductance in Nanowires”, E. N. Bogachek, A. G. Scherbakov, and U. Landman, Phys. Rev. B, October (1999), in press.

4. Interactions/Transitions

(a) Invited Talks

Invited Speaker, Nato Advanced Workshop on "Nanowires", Sept. 1996.
Plenary Lecture in "Quantum Optics and Clusters", Joint Polish-German Conference, Katowica, Poland, September, 1996.
Invited Speaker, American Vacuum Society Annual Meeting, Philadelphia, Oct. 1996.
Invited Speaker, "Friction, Arching, Contact Dynamics", Julich, Germany, Oct. 1996.

Invited Speaker, MRS Annual Meeting, Boston, Nov. 1996.
Invited Speaker, "Workshop on Total Energy and Force Computations", Trieste, Italy, January 1997.
Invited Speaker, German Physical Society Annual Meeting, Munster, Germany, March 1997.
Invited Speaker, NSF Workshop on "Nanoscience and Technology", Washington, D.C., May 1997.
Invited Speaker, "Nato Forum on Nanoscale Science and Technology", Toledo, Spain, May 1997.
Invited Speaker, "European Materials Research Society," Strassburg, France, June 1997.
Invited Speaker, "Quantum Theory Symposium", Raleigh, N. C., June 1997.
Invited Speaker, "AFOSR/ONR Symposium on Tribology", Dayton, Ohio, June 1997.
Plenary Speaker, Conference on "Oriented Molecules", Bielefeld, Germany, July 1997.
Invited Speaker, Gordon Conference on "Organic Films", Salva Regina, July 1997.
Invited Speaker, "STM 97", Hamburg, Germany, July 1997.
Discussion Leader, Gordon Conference on "Clusters and Nanoparticles", July 1997.
Invited Speaker, Gordon Conference on "Gas Surface Dynamics", August 1997.
Plenary Speaker, "Physics Computing '97", Santa Cruz, California, August 1997.
Invited Speaker, "National School on Materials Science", Genova, Italy, October 1997.
Invited Speaker, "Advancing Frontiers of Condensed Matter Science", Philadelphia, Oct. 1997.
Invited Speaker, "Computational Physics", Vanderbilt, Nashville, Tenn., November 1997.
Invited Speaker, "Confined Liquids", Ein-Gedi, Israel, December 1997.
Invited Speaker, "Large-Scale Computing for Nanoscale Systems", Pisa, Italy, December 1997.
Keynote Speaker, The Swedish Agency for Strategic Research, Scientific Consortia Meeting, Stockholm, January 1998.
Invited Speaker, APS Meeting, Los-Angeles, March 1998.
Invited Speaker, ACS Meeting, Dallas, Texas, April 1998.
Invited Speaker, "Cluster-Surface Collisions", Corsica, Italy, May 1998.
Keynote Speaker, Nanotribology, Genova, Italy, June 1998.
Invited Speaker, (two lectures) "Workshop on Clusters", University of Washington, Seattle, July 1998.
Invited (keynote) Speaker, Gordon Conference on "High-Temperature Materials", New Hampshire, July 1998.
Invited Speaker, Material Research Society Meeting, Boston, November 1998.
Invited Speaker, JRCAT (Joint Research Centr for Atom Technology), Conference on "Atomic Scale Manipulation", Tskuba, Japan, January 1999.
Invited Speaker, "Workshop on Mesoscopic Systems", Paris, France, March 1999.
Invited Speaker, Conference on "Nanocomposite Materials: Design and Applications", Ayleska, Alaska, March 1999.
Invited Speaker, (J. Gao), American Physical Society, Atlanta, March 1999.
Plenary Speaker, "International Conference on Metallurgical Coatings and Thin Films", San Diego, April 1999.
Invited Lecturer, (3 lectures), "Quantum Mesoscopic Phenomena and Mesoscopic Devices in Microelectronics", NATO Advanced Study Institute, Ankara, Turkey, June 1999.

Keynote Speaker, Conference on "Nanoscience", Hong Kong, July 1999.
Invited Speaker, Gordon Conference on "Clusters and Nanostructures", New London, CT, July 1999.
Invited Speaker, American Chemical Society, New Orleans, August 1999.

(b) A figure from our work on nanotribology appeared as a cover illustration of the July 1999 issue of Physics Today.

Our work had been reviewed in several scientific magazines such as Science News, The Bulletin of the Material Research Society, and in trade magazines.

4. Honors and Professional Appointments

- U. Landman was elected as a Distinguished Lecturer of the American Vacuum Society (1999).
- U. Landman served as a co-director of a Nato Advanced Research Workshop on "Nanowires", (Spain, 1996).
- U. Landman has been reappointed to the Editorial Board of the Journal of Physical Chemistry.

5. Personnel

Supported by the Grant

Uzi Landman - Callaway Chair in Computational Materials Science and Regents' Professor
W. D. Luedtke - Senior Research Scientist
J. Gao - Senior Research Scientist
E. Ringer - Graduate Student (received his Ph.D. Degree, Spring 1999).

Associated with the Research Effort:

C. L. Cleveland - Senior Research Scientist
H. Häkkinen - Senior Research Scientist