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PROJECT ADMINISTRATION DATA SHEET

[XX] ORIGINAL [ ] REVISION NO. ____

Project No. G-41-619 (R6132-0A0) GTRC/GIT DATE 5 / 13 / 86

Project Director: Uzi Landman, Martin Ribarsky, Ward Winer School/XXX Physics

Sponsor: National Science Foundation

Type Agreement: Grant No. MSM-8611257

Award Period: From 5/1/86 To 10/31/87 (Performance) 1/31/88 (Reports)

Sponsor Amount:	This Change	Total to Date
Estimated: $		$ 29,994
Funded: $		$ 29,994

Cost Sharing Amount: $ 3,042 Cost Sharing No: G-41-361

Title: Theoretical Studies of the Microscopic Mechanisms of Friction and Wear

ADMINISTRATIVE DATA

OCA Contact John B. Schonk X4820

1) Sponsor Technical Contact:	2) Sponsor Admin/Contractual Matters:
Said Jahanmir	Shirley A. Woods
National Science Foundation	National Science Foundation
ENG/MSM	DGC/ENG
Washington, DC 20550	Washington, DC 20550
202/357-9542	202/357-9626

Defense Priority Rating: N/A Military Security Classification: N/A

(or) Company/Industrial Proprietary: N/A

RESTRICTIONS

See Attached NSF Supplemental Information Sheet for Additional Requirements.

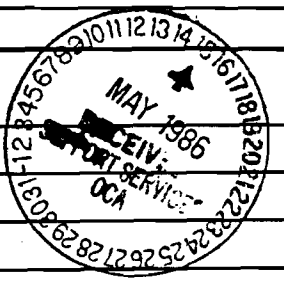
Travel: Foreign travel must have prior approval — Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with GIT

COMMENTS:

No funds may be expended after 10/31/87

*Includes a 6-month no cost flexibility period.



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GEORGIA INSTITUTE OF TECHNOLOGY OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 3/10/88

Project No. G-41-619 School/~~Lab~~ Physics

Includes Subproject No.(s) N/A

Project Director(s) M. W. Ribarsky GTRC/~~GTI~~

Sponsor National Science Foundation

Title Theoretical Studies of the Microscopic Mechanisms of Friction and Wear

Effective Completion Date: 10/31/87 (Performance) 1/31/88 (Reports)

Grant/Contract Closeout Actions Remaining:

- [ ] None
- [ ] Final Invoice or Copy of Last Invoice Serving as Final
- [ ] Release and Assignment
- [X] Final Report of Inventions and/or Subcontract:
  Patent and Subcontract Questionnaire sent to Project Director [X]
- [ ] Govt. Property Inventory & Related Certificate
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Continues Project No. Continued by Project No.

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APPENDIX VII

NATIONAL SCIENCE FOUNDATION
Washington, D.C. 20550

FINAL PROJECT REPORT
NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

PART I–PROJECT IDENTIFICATION INFORMATION

1. Institution and Address	2. NSF Program	3. NSF Award Number
Georgia Institute of Technology Atlanta, Georgia 30332	Tribology/ Engineering Directorate	MSM-861 11257
	4. Award Period From 5/1/86 To 4/30/87	5. Cumulative Award Amount $ 29,994

6. Project Title

Theoretical Studies of Microscopic Mechanisms of Friction and Wear

PART II–SUMMARY OF COMPLETED PROJECT *(FOR PUBLIC USE)*

The objectives of the project were to provide the foundations for computer simulations of the microscopic processes that govern interfacial friction and wear phenomena and to implement and demonstrate the applicability of such theoretical methods to the elucidation of the mechanisms and to the identification of the material parameters (such as cohesive energies, atomic sizes and interatomic distances) underlying these processes. We developed a computational strategy for studies of material interfaces under non-isotropic stress and have developed the computer codes and analysis routines for molecular dynamics simulations of such systems. In these simulations the classical equations of motion of a collection of particles interacting via prescribed potentials and influenced by external stresses are numerically solved and the data analyzed to obtain energetic, structural and dynamic information on refined microscopic spatial and temporal scales. Using generic interatomic potentials we have used a microscopic formulation which allows treatment of materials undergoing finite deformations. We found that when a shear stress is applied to a system in which the two interfacing materials differ in cohesive strength only, plastic deformation and eventual yield (and flow) is preceded by a sequence of structural transformation occuring in the softer material in a region separated from the equilibrium interface by a narrow (few atomic layers) transfer region. Furthermore, for fcc materials we found that these structural transformations consist of stacking fault formation and slip. The critical stresses at which the material transforms and eventually yields depend upon the crystallographical characteristics and ambient thermal conditions (i.e., thermally adiabatic versus isothermal conditions). In addition we found that the critical stresses and the stress relief and frictional resistance mechanisms depend on the atomic size mismatch between the interfacing substrate and solid lubricant. In addition to the above we have initiated studies of the interaction between atomic size tips and solid substrates, (Si) suggesting the use of atomic-force-microscopy in tribological studies and demonstrating the effect of the dynamical tip-substrate interaction on the data. Our simulations demonstrate the feasibility of modeling tribological phenomena on a microscopic scale and the wealth of structural and dynamical data which can be obtained via such studies.

PART III–TECHNICAL INFORMATION *(FOR PROGRAM MANAGEMENT USES)*

1. ITEM *(Check appropriate blocks)*	NONE	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM	
				Check (√)	Approx. Date
a. Abstracts of Theses					
b. Publication Citations		X	X		
c. Data on Scientific Collaborators					
d. Information on Inventions					
e. Technical Description of Project and Results			X		
f. Other *(specify)*					

2. Principal Investigator/Project Director Name *(Typed)*	3. Principal Investigator/Project Director Signature	4. Date
Uzi Landman, Martin W. Ribarsky		2/10/88

NSF Form 98A (3-83) Supersedes All Previous Editions

Form Approved OMB No. 3145-0058

PART IV - SUMMARY DATA ON PROJECT PERSONNEL

NSF Division _____

The data requested below will be used to develop a statistical profile on the personnel supported through NSF grants. The information on this part is solicited under the authority of the National Science Foundation Act of 1950, as amended. All information provided will be treated as confidential and will be safeguarded in accordance with the provisions of the Privacy Act of 1974. NSF requires that a single copy of this part be submitted with each Final Project Report (NSF Form 98A); however, submission of the requested information is not mandatory and is not a precondition of future awards. If you do not wish to submit this information, please check this box ☐

Please enter the numbers of individuals supported under this NSF grant.
Do not enter information for individuals working less than 40 hours in any calendar year.

*U.S. Citizens/ Permanent Visa	PI's/PD's		Post-doctorals		Graduate Students		Under-graduates		Precollege Teachers		Others	
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American Indian or Alaskan Native												
Asian or Pacific Islander												
Black, Not of Hispanic Origin												
Hispanic												
White, Not of Hispanic Origin	✓											
Total U.S. Citizens	2											
Non U.S. Citizens												
Total U.S. & Non-U.S. ..												
Number of individuals who have a handicap that limits a major life activity.												

*Use the category that best describes person's ethnic/racial status. (If more than one category applies, use the one category that most closely reflects the person's recognition in the community.)

AMERICAN INDIAN OR ALASKAN NATIVE: A person having origins in any of the original peoples of North America, and who maintains cultural identification through tribal affiliation or community recognition.

ASIAN OR PACIFIC ISLANDER: A person having origins in any of the original peoples of the Far East, Southeast Asia, the Indian subcontinent, or the Pacific Islands. This area includes, for example, China, India, Japan, Korea, the Philippine Islands and Samoa.

BLACK, NOT OF HISPANIC ORIGIN: A person having origins in any of the black racial groups of Africa.

HISPANIC: A person of Mexican, Puerto Rican, Cuban, Central or South American or other Spanish culture or origin, regardless of race.

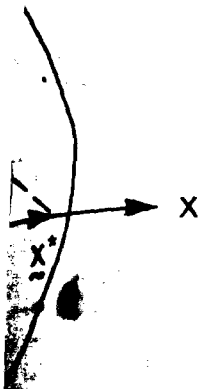
WHITE, NOT OF HISPANIC ORIGIN: A person having origins in any of the original peoples of Europe, North Africa or the Middle East.

THIS PART WILL BE PHYSICALLY SEPARATED FROM THE FINAL PROJECT REPORT AND USED AS A COMPUTER SOURCE DOCUMENT. DO NOT DUPLICATE IT ON THE REVERSE OF ANY OTHER PART OF THE FINAL REPORT.

4.19 MICROSCOPIC MECHANISMS OF TRIBOLOGICAL AND WEAR PROCESSES: MOLECULAR DYNAMICS SIMULATIONS

Martin W. Ribarsky and Uzi Landman

Although tribological phenomena are an everyday experience and have been observed and studied for a very long time [1], a detailed microscopic theory of tribological phenomena is lacking. Nevertheless a large body of empirical data has been collected and some phenomenological models have been developed [2]. The major reasons, from a theorist's perspective, for this state of affairs may be attributed to: (i) the complexity of the phenomena, which involve processes occurring in materials under stress, the generation and propagation of defects, large structural deformations and properties of systems beyond the elastic regime, (ii) the nature of available experimental data, which until fairly recently was not obtained under controlled conditions on compositionally and structurally well characterized samples. Recent advances in computer simulation methods [3] and the advent and application of surface science experimental probes provide the impetus for the development of fundamental models, on the atomic scale, of tribological and wear phenomena. In this note we outline our recent investigations in this area using molecular-dynamics (MD) simulations, and demonstrate the potential of such investigations towards the development of a microscopic understanding of the physical processes which underly these phenomena.



METHOD

Computer simulations, where the evolution of a physical system is simulated with refined temporal and spatial resolution, via direct numerical solution of the equations of motion of a system of interacting particles, are in a sense computer experiments which open new avenues in investigations of the microscopic origins of material phenomena [3]. In its simplest form [4], the interaction between particles i and j is described by a pair potential $\phi(r_{ij})$ where $r_{ij} = |\vec{r}_i - \vec{r}_j|$, and the classical equations of motion for a system of N particles, of masses M_i, are given by

$$M_i \frac{d^2\vec{r}_i}{dt^2} = -\sum_{j=i}^{N} \frac{\partial\phi(r_{ij})}{\partial\vec{r}_i} \quad . \tag{1}$$

Practical considerations restrict the number of dynamical particles contained in the calculational cell to be of the order of 10^3-10^4, and the simulation of the extended system is achieved via the employment of periodic boundary conditions. For exploration of the elastic behavior of solids and phenomena which may involve external stresses, volume changes, shape and structural deformations, it is important that the variables which determine the volume and shape of the calculational cell will be allowed to respond dynamically. In our calculations we have used a

newly developed method [5] which allows for the above dynamical considerations.

MODEL CALCULATIONS

To illustrate the method we have constructed a model system consisting of 1200 (or 1260) particles in the calculational cell (which is periodically repeated), interacting via 6-12 Lennard-Jones potentials,

$$\phi_{\alpha\beta}(r) = 4\epsilon_{\alpha\beta}\left[(\sigma_{\alpha\beta}/r)^{12} - (\sigma_{\alpha\beta}/r)^{6}\right] \qquad (2)$$

with $\sigma_{\alpha\beta} = (\sigma_{\alpha\alpha}+\sigma_{\beta\beta})/2$ and $\epsilon_{\alpha\beta} = (\epsilon_{\alpha\alpha}\,\epsilon_{\beta\beta})^{1/2}$. The bottom half of the system (α) was characterized by an interaction strength parameter $\epsilon_{\alpha\alpha} = 2\epsilon_{\beta\beta}$, where $\epsilon_{\beta\beta}$ determines the interaction strength in the other part of the system (β). In this arrangement the soft material (β) may be viewed as a solid lubricant, whose melting point is half that of the surrounding material. In order to isolate the effect of interaction strength from other material parameters we have taken $\sigma_{\alpha\alpha} = \sigma_{\beta\beta}$. In the following we use reduced units [6] where energy (and temperature) are expressed in units of $\epsilon_{\alpha\alpha}$, length in units of $\sigma_{\alpha\alpha}$ and the time unit (t.u.) is $(m_\alpha/\epsilon_{\alpha\alpha})^{1/2}\sigma_{\alpha\alpha}$, (the integration time-step Δt was 0.0075t.u.). Two series of studies were conducted: (1) The interface between the hard (α) and soft (β) components of the system was in the (001) plane, $N_{layer} = 20$, $N = 1200$; layers 1-10 of material α and 11-20 of material β. (2) The interface was in the (111) plane, $N_{layer} = 18$, $N = 1260$; interface between layers 9 and 10. At the start of the calculations the systems were equilibrated at a reduced temperature $T \sim 0.11$ (about $T^{(\alpha)}_{melting}/6$). Subsequently, a load [6] of 0.5 was imposed along the direction normal to the interface. Following equilibration under load, the system was subjected to shear stress (in the <110> direction for the (001) interface, and in the $\langle 1,\bar{1},0\rangle$ direction for the (111) interface) which was increased gradually until the system failed. Special care was taken to determine the yield stress, σ_c. In addition, simulations at constant external shear-stress were conducted. In this report we restrict ourselves to thermally isolated (adiabatic) systems.

From the temporal evolution of the particle trajectories, generated via the integration of the equations of motion, the internal stress tensor in the system can be calculated [7]. The time evolution of the internal stress in layers, σ_{xz} (i.e., along the <110> direction), for a fixed external stress of 1.9375 ($\sigma_c = 1.925 \pm 0.012$), just before and during yield for the (001) system, is shown in Fig. 1a. We observe that variations in the internal stresses start in the soft material, in a region removed from the interface (originally located between layers 10 and 11), i.e., layers 13-15, while layers 11 and 12 which are adjacent to the interface are pinned, at the onset of yield, by their interaction with the hard substrate.

This sequence of events is further demonstrated by the particle trajectories

shown in Fig. 2. Here, the initial position of an atom is at the center of the circle, from where the indicated trajectory develops. These trajectories correspond to the time interval 232-235 t.u. (see Fig. 1a). As seen, while layers 11 and 12 move uniformly with layer 10 of the substrate, deeper layers in the soft material do not. Note that the movement in either direction tends to involve entire rows rather than having motion in several directions for some rows. In fact, layers 16, 17, 18, 19, and 20 viewed together show that, in successive planes, one new row at a time joins in the leftward movement until all rows are moving to the left by layer 20. A geometrical analysis of the slip in layers 16 through 20 reveals that two intersecting slip planes are involved: $\{1\bar{1}1\}$ and $\{\bar{1}11\}$. Thus, even though the system was sheared along the {001} plane in the (110) direction, the slip occurred in {111}-type planes. This is just the expected experimental result since all methods consistently indicate that {111}-type planes in (110) directions are the major operative slip systems in FCC structures. The deformation of the system is accompanied by an increase in temperature (see Fig. 1b), which "autocatalyzes" plastic deformation and eventual total yield. The coefficient of friction which is obtained from these calculations σ_c/load = 4, which is of the order of typical values for the static coefficient for clean metal surface in contact in vacuum.

To demonstrate the dependence of the mechanisms of deformation and transformation on the crystallography of the interface, we have performed similar simulations for a system in which the interface was in the (111) plane. We find that under adiabatic conditions this system yields at $\sigma_c = 0.859$. When the system is sheared in the $\langle 1\bar{1}0\rangle$ direction, under adiabatic conditions, below the yield stress, it slips at $\sigma_s = 0.797 \pm 0.016$ generating stacking faults in the soft (lubricant) material. Allowing the system to relax under σ_s and then increasing the imposed stress, the system yields at $\sigma_c = 0.859 \pm 0.016$. Similar calculations for a system under isothermal conditions exhibit a slip stage occurring at $\sigma_s = 0.85 \pm 0.025$ and eventual yield at $\sigma_c = 0.97 \pm 0.03$. The system in contact with a heat reservoir (isothermal) withstands higher shear stresses as compared to the adiabatic case, since in the latter case the heat which is generated in the course of the deformation of the system is utilized to overcome potential barriers for sliding, while in the former case this heat is dissipated to the reservoir and higher shear stresses are necessary to bring about a similar effect. In addition, we note the difference between the critical stresses σ_c, for the (111) and (001) interface orientations. The degree of detail afforded by the MD simulations is further demonstrated by the selected particle configurations shown in Fig. 4, for the adiabatic (111) interface, exhibiting the formation of a stacking fault in the soft material. For this system the original interface is between layers 9 and 10 and the stacking fault is generated at layers 12 and 13 (see Fig. 3, in which a slice of the system viewed along the $\langle 10\bar{1}\rangle$ direction, before and after the generation of the stacking fault, is shown). The sequence of configurations shown in

Fig. 4 (separated by 170 Δt) show layers 12 and 13 starting at registry (4a) and moving out of registry and into new equilibrium positions Fig. 4c), generating a stacking fault.

While in the above we focused on systems characterized by interfaces with differing interaction strengths, the effect of other material parameters such as lattice parameter mismatch, covalent (directional) bonding and long-range interactions (as found in ionic materials) as well as effects due to ambient conditions such as shear rates, and normal load values, are under investigation. Finally, while we found evidence for the generation of dislocations in our simulations, the full development of these extended defects would require simulation for larger systems.

ACKNOWLEDGEMENTS

This work is supported by NSF Grant No. MSM-8611257 and by a contract from the Hughes Aircraft Company. Partial support was provided by U.S. DOE Grant No. F505-86ER45234.

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5. "Polymorphic Transitions in Single Crystals: A New Molecular Dynamics Method," M. Parrinello and A. Rahman, *Journal of Applied Physics, 52*, 7182-7190 (1981).
6. If we choose interaction parameters which correspond to the cohesive energy and lattice constant of Nickel ($\epsilon = 3.64\times10^{-13}$erg, $\sigma = 2.49$Å and $M = 9.75\times10^{-23}$g) a reduced temperature $T = 0.11$ corresponds to 300°K, the melting temperature $T_m = 0.7$ to 2000°K, the reduced unit of stress or load to 2.4×10^{7}g/cm^2 (or 2.4×10^{10} dynes/cm^2) and the time-unit corresponds to 4.1×10^{-13} sec. Time expressed in terms of the above time unit is denoted by t*.
7. "Local Structural Fluctuations in Amorphous and Liquid Metals: A Simple Theory of the Glass Transition," T. Egami and D. Srolovitz, *Journal of Physics of Fluids, 12*, 2141-2163 (1982).

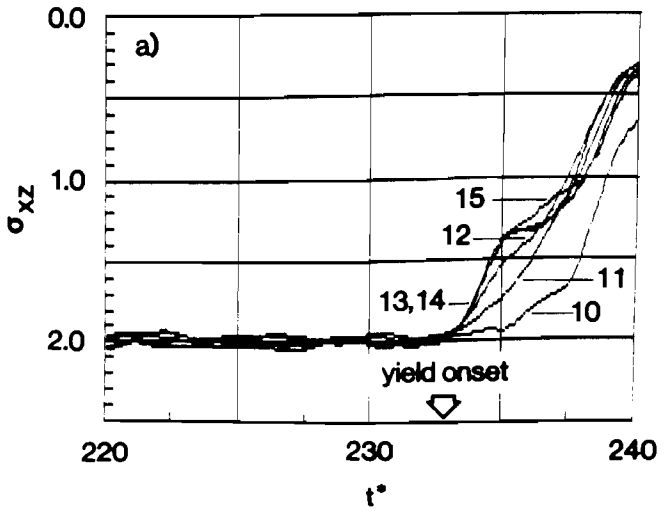

Fig. 1a. Internal shear stress per layer in the same direction and along the same plane as the external stress, σ_{ext} = 1.9375, versus reduced time. Note the initiation of response to the applied stresses in layers 13-15.

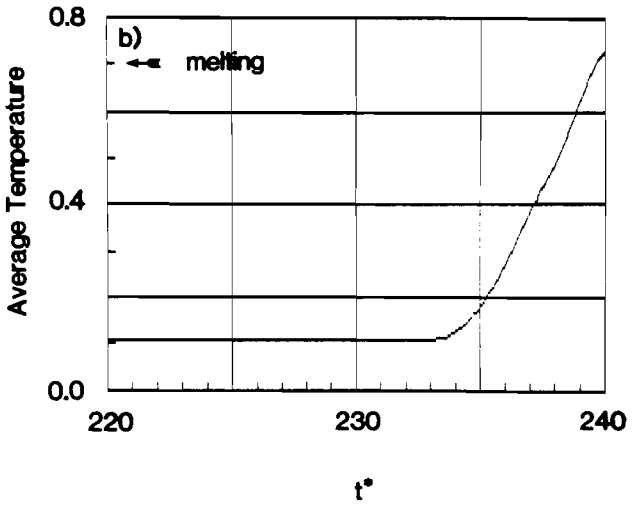

Fig. 1b. Temperature for the total system versus reduced time.

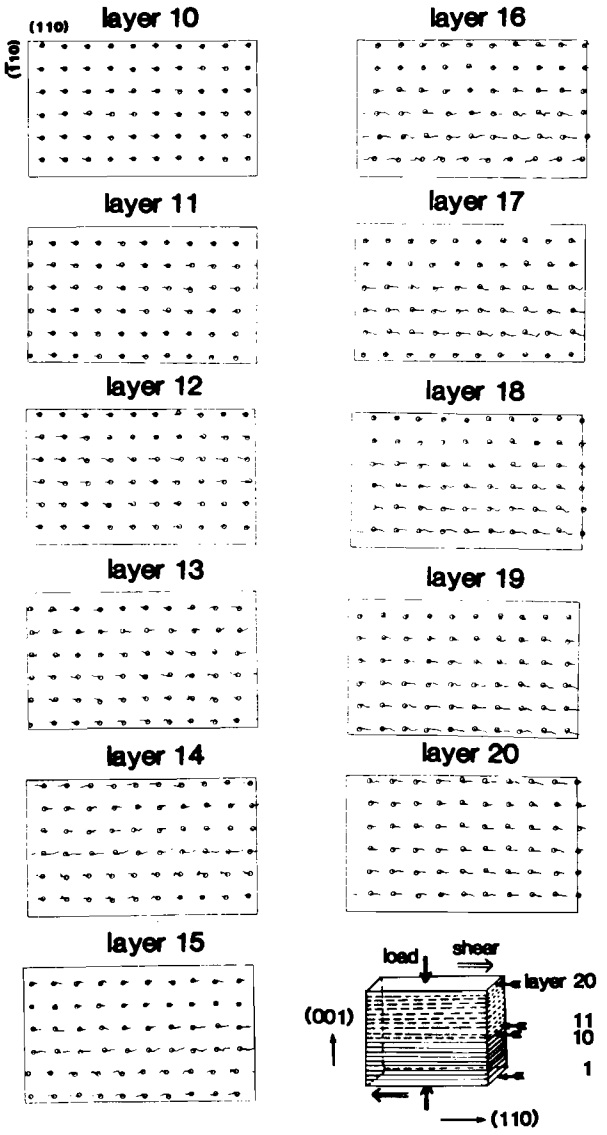

Fig. 2. Atomic trajectories for successive {001} layers. The hard-soft interface is between layers 10 and 11. The trajectories shown are for σ_{ext} = 1.9375 at t^* = 232-235 t.u. A schematic of the calculational cell is shown at the bottom right hand side.

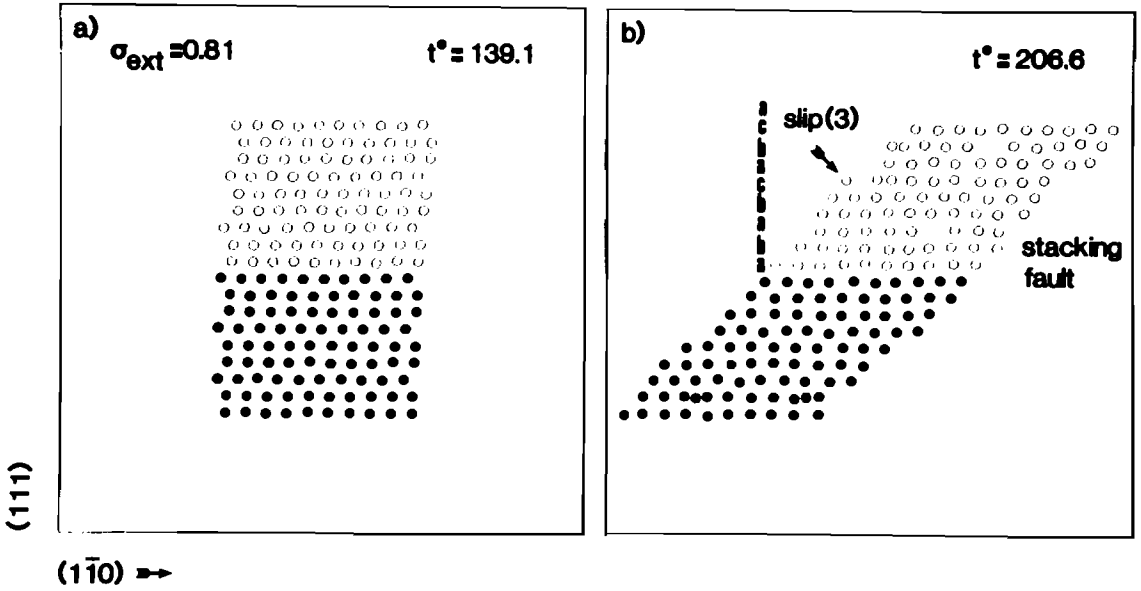

Fig. 3. Atomic trajectories for a central slice of the {111} system at σ_{ext} = 0.81. a) Before slip and b) after slip. A stacking fault occurs in layers 10-13, and layer 15 slips 3 rows to the left.

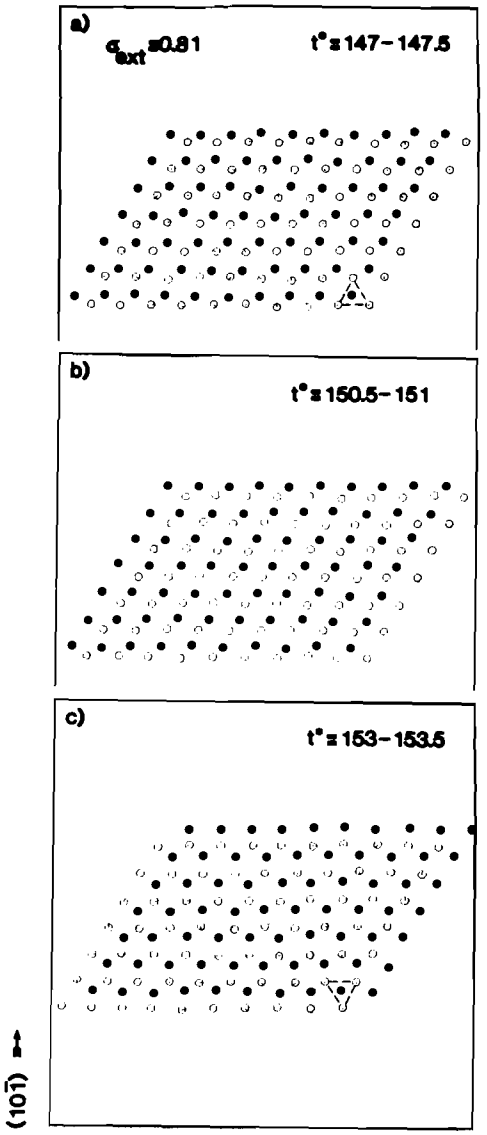

Fig. 4. Layers 12 (shaded circles) and 13 from the {111} system during the formation of the stacking fault. a) Before the stacking fault forms, the registry between layers is indicated by the dotted lines. b) Midway through stacking fault formation. c) The layers have moved to a new registry, indicated by the dotted lines.

F.F. Ling C.H.T. Pan

Approaches to Modeling of Friction and Wear

Proceedings of the Workshop on the Use of
Surface Deformation Models to Predict Tribology Behavior
Columbia University in the City of New York
December 17–19, 1986

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