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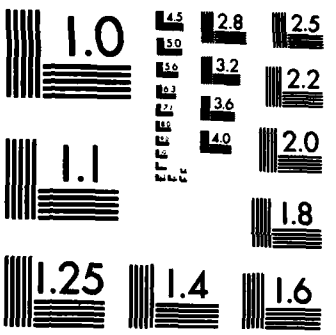

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Abstract

Structural, thermodynamic and mechanical properties of bicrystals have been studied using molecular dynamics and Monte Carlo simulation. A grain boundary melting transition in a two-dimensional system has been observed. Atomic diffusion along grain boundaries was investigated by following in detail the migration of a vacancy initially introduced into the bicrystal. The activation energy for vacancy migration in iron has been determined, and thermal activation of Frenkel pairs in the grain boundary core was observed.

Structural phase transformation in stressed solids has been studied using an extended Monte Carlo method. Stress-strain relations obtained for iron showed the existence of bcc $\leftrightarrow$ fcc transition under tension or compression.

Dynamical properties of a one-dimensional nonlinear lattice (the U^4-lattice) have been analyzed in terms of kink propagation and damping and kink diffusion. Both perturbation theory and molecular dynamic calculations were carried out.

Computer Simulation Studies of Grain Boundary Systems and Molecular Solids

FINAL REPORT

Sidney Yip

April 19, 1983

U.S. Army Research Office

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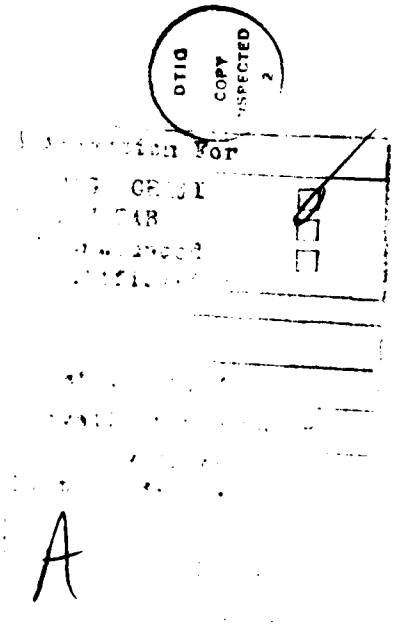

CONTENTS

I. INTRODUCTION

This report summarizes the work performed during the contract period, January 1, 1978 through January 31, 1983. The total funding was $222,485. The personnel supported were one principal investigator and six graduate students who received five Ph.D. and one M.S. as terminal degrees.

II. DESCRIPTION OF PROBLEMS STUDIED

The basic objective of the project was to study by means of the discrete particle simulation techniques of molecular dynamics and Monte Carlo several problems in materials properties and behavior of solids. These problems involved highly nonlinear, nonhomogeneous, or nonequilibrium processes which were difficult to analyze analytically or to measure experimentally. In each case, appropriate computer simulation programs were developed and results obtained which not only established the validity of the simulation modeling approach, but also provided detailed information and insight at the molecular level of materials behavior.

Structural Stability of High-angle Grain Boundary at Elevated Temperatures and Point Defect Motions in Self-diffusion

Grain boundary structures are often determined by static calculation in which the potential energy is minimized. We have studied by molecular dynamics the structural stability of such a configuration in the case of a $\Sigma=5$ ($\theta=36.87°$) [001] tilt boundary in bcc iron when the system is heated up to about two-thirds of melting temperature and beyond. The thermal motion of a vacancy, initially introduced into a statically relaxed position, was observed in sufficient detail and duration to determine the activation energy for migration and the various jump frequencies to sites in the grain boundary core. The simulation also provided data on thermal activation of Frenkel pairs in the core and the mobility of the interstitials thus produced. In another study, simulation was carried out on a two-dimensional bicrystal, $\Sigma=7$ ($\theta=38.21°$), to investigate the existence of a grain boundary phase transition. In addition, grain boundary-point defect interactions were studied by Monte Carlo simulation.

Crack Tip Processes and Ductile/Brittle Behavior in Mode I Fracture

In atomistic study of crack propagation, it is essential to treat properly the boundary between the interior (discrete) region containing the crack tip and the exterior (elastic continuum) region

where the stress is being applied. Existing methods are not satisfactory because the boundary is not sufficiently flexible to allow nucleation of dislocations at the tip and subsequent propagation away from the crack. A new method was developed which replaces the exterior region by appropriate stresses on the boundary and which allows the boundary atoms to move freely otherwise. This method was incorporated in a molecular dynamics investigation of crack extension (mode I fracture) in bcc iron and fcc copper by determining the critical stress intensity factor and detailed stress and strain distributions surrounding the crack.

Thermal Ignition of an Exothermically Reacting Fluid

A basic problem in the theory of thermal explosion is the determination of the critical condition under which the temperature of a piece of material undergoing self heating rises precipitously. Using a molecular dynamics model of two-dimensional fluids of hard sphere particles capable of collision-induced exothermic reactions, we have investigated the critical properties of slabs of varying sizes and densities, results which can be compared with predictions of classical continuum theory. Other results include the induction period and temperature profiles.

Propagation and Diffusive Motions of Kink Structure in a One-dimensional Nonlinear Lattice

A linear chain of atoms coupled to nearest neighbors by harmonic forces but each is also subjected to a double-well potential (the U^4-lattice model) can exhibit highly nonlinear dynamical behavior. In particular, there exist atom configurations where atoms oscillating in the left side of their double wells are separated by a "domain wall" or "kink" from those oscillating in the right side of the potential wells. We have studied the propagation and damping of such a kink in various velocity regimes using molecular dynamics simulation and perturbation theory analysis. Simulation data on kink diffusion in a thermal lattice have been obtained at various temperatures.

Structural and Mechanical Properties of Stressed Crystals and Bicrystals

We have extended the conventional Monte Carlo method to the simulation of stressed solids. Structural phase transitions which occurred in cubic crystals under uniaxial tensions or compressions have been observed through a detailed mapping of stress-strain curves for bcc iron and fcc Ni. Similar, but less extensive, results were obtained for bicrystals of a noble-gas element.

III. SUMMARY OF MOST IMPORTANT RESULTS

In each of the areas of investigation described above we have demonstrated that atomistic simulation can indeed provide unique and valuable information. The most significant results that emerged are the following:

1. Observation of vacancy jumps in a bicrystal of bcc iron and demonstration that vacancy exchange is the dominant mechanism for fast diffusion along grain boundaries. Related results are the determination of activation energy for vacancy migration in bcc iron and the observation of thermal activation of boundary interstitials which were found to be largely immobile [1,2].*

2. Observation of grain boundary phase transformation in a two-dimensional bicrystal by molecular dynamics simulation at constant pressure [8].

3. Development of a new boundary condition for modeling a system of discrete atoms surrounded by an appropriately stressed elastic medium, and demonstration that crack extension occurs in bcc iron without dislocation emission and in fcc copper with dislocation emission [3].

4. Demonstrated ability to simulate thermal ignition processes in reacting fluids and quantitative test of classical continuum theory of thermal explosion. Feasibility of studying effects of fluctuations in the vicinity of criticality is established [4].

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*Numbers in brackets refer to published work in the List of Publications.

5. Observation of finite-temperature martensitic (Bain) transformation bcc ↔ fcc in iron by Monte Carlo simulation. Related results of stress-induced structural transformations in solids and mechanical properties of stressed bicrystals.

6. Determination of grain boundary interactions with vacancies and impurities.

7. Development of a new dynamical theory of kink propagation and damping in one-dimensional nonlinear lattices and study of kink diffusion by molecular dynamics simulation.

IV. List of Publications

1. G.H. Bishop, R.J. Harrison, T. Kwok and S. Yip, "Simulation of Grain Boundaries at Elevated Temperatures by Computer Molecular Dynamics," in Progress in Materials Science, Chalmers Anniversary Volume, ed. by J.W. Christian, P. Haasen and T.B. Massalski (Pergamon Press, Oxford, 1981), p. 49.

2. T. Kwok, P.S. Ho, S. Yip, R.W. Balluffi, P.D. Bristowe and A. Brokman, "Evidence for Vacancy Mechanism in Grain Boundary Diffusion in Iron: A Molecular Dynamics Study," Physical Review Letters 47, 1148 (1981).

3. R.W. Balluffi, T. Kwok, P.D. Bristowe, A. Brokman, P.S. Ho and S. Yip, "Determination of Vacancy Mechanism for Grain Boundary Self-Diffusion by Computer Simulation," Scripta Metallurgica 15, 951 (1981).

4. D.P. Chou and S. Yip, "Computer Molecular Dynamics Simulation of Thermal Ignition in a Self-Heating Slab," Combustion and Flame 47, 215 (1982).

5. G.H. Bishop, R.J. Harrison, T. Kwok and S. Yip, "Computer Molecular Dynamics Simulation Studies of Grain Boundary Structures: I. Observations of Coupled Sliding and Migration in a Three-dimensional Simulation," Journal of Applied Physics 53, 5596 (1982).

6. G.H. Bishop, R.J. Harrison, T. Kwok and S. Yip, "Computer Molecular Dynamics Simulation of Grain Boundary Structures: II. Migration, Sliding and Annihilation in a Two-Dimensional Solid," Journal of Applied Physics 53, 5609 (1982).

7. B. deCelis, A.S. Argon and S. Yip, "Molecular Dynamics Simulation of Crack Tip Processes in Alpha Iron and Copper," Journal of Applied Physics (1983), in press.

8. F. Carrion, G. Kalonji and S. Yip, "Evidence for Grain Boundary Phase Transition in a 2D Bicrystal," Scripta Metallurgica, submitted.

9. J.A. Combs and S. Yip, "Single Kink Dynamics in a One-Dimensional Atomic Chain," Physical Review B, submitted.

10. J.A. Combs and S. Yip, "Molecular Dynamics Study of Lattice Kink Diffusion," Physical Review B, submitted.

11. E. Leutheusser, D.P. Chou and S. Yip, "Van Hove Self-correlation Function of a Hard-disk Fluid," Journal of Statistical Physics (1983), in press.

6 manuscripts for journal publication are still under preparation.

V. PARTICIPATING SCIENTIFIC PERSONNEL

All the personnel who participated in the contract research are listed below along with the period of participation. Graduate degrees conferred are indicated along with the thesis title. In addition, it should be noted that the published work involved a number of other collaborators, Drs. G.H. Bishop and R.J. Harrison (Army Materials and Mechanics Research Center, Watertown, MA), Dr. Paul S. Ho (IBM Watson Research Center, Yorktown Heights, NY), Professor R.W. Balluffi, Professor G. Kalonji, Drs. P.D. Bristowe and A. Brokman (Department of Materials Science and Engineering, MIT), and Professor A.S. Argon (Department of Mechanical Engineering, MIT).

Principal Investigator

Sidney Yip (1/78 - 1/83)

Research Assistants and Graduate Students

Dong-Pao Chou (1/78 - 8/81)

"Molecular Dynamics Simulation of Self-diffusion in Hard-disk Fluids," Nuclear Engineer's Thesis (1980)

"Continuum Theory and Molecular Dynamics Simulation of Temperature Instabilities in a Self-heating Slab," Ph.D. Thesis (1981).

Thomas Kwok (1/78 - 9/81)

"Computer Molecular Dynamics Studies of Two-dimensional Grain Boundary Crystals," M.S. Thesis (1978).

"Computer Simulation of Vacancy Motions and Diffusion Kinetics in a bcc Grain Boundary," Ph.D. Thesis (1981).

J. Andrew Combs (1/78 - 9/81)

"Theory and Simulation of U^4-lattice Kinks in a One-dimensional Atomic Chain," Ph.D. Thesis (1981).

Benito de Celis (1/78 - 5/82)

"Molecular Dynamics Simulation Studies of Fracture in Two Dimensions," Nuclear Engineer's Thesis (1980).

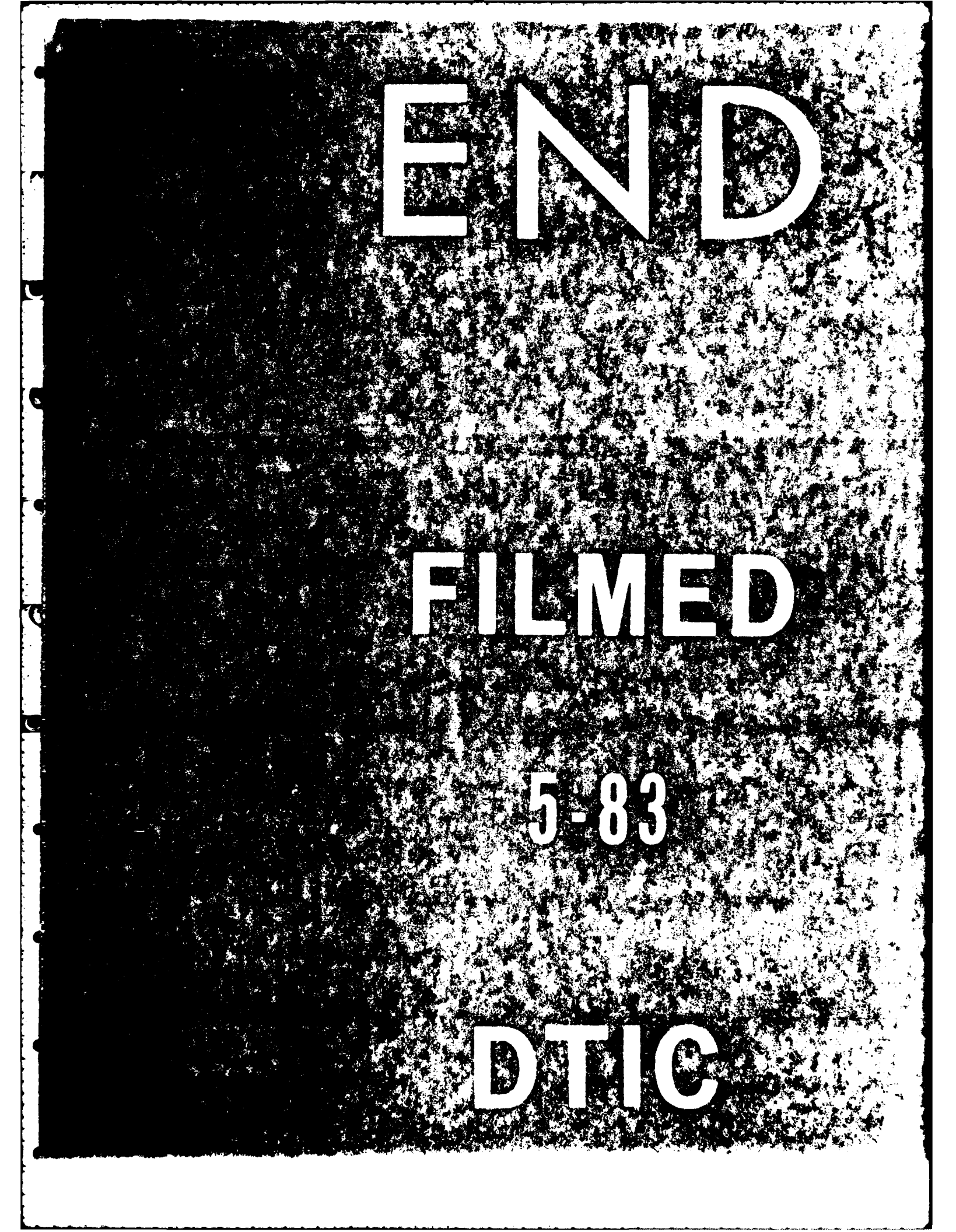
"Molecular Dynamics Simulation Studies in Fracture Mechanics," Ph.D. Thesis (1982).

Francisco Carrion (9/81 - 8/82)

"Molecular Dynamics Simulation Study of Structural Stability and Melting of Two-dimensional Crystals," M.S. Thesis (1982).

Reza Najafabadi (2/80 - 1/83)

"Monte Carlo Simulation of Structural and Mechanical Properties of Crystal and Bicrystal Systems at Finite Temperature," Ph.D. Thesis (1983).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