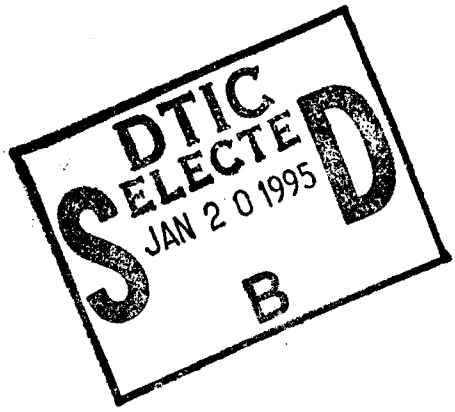
RL-TR-94-210
Final Technical Report
November 1994

MOLECULAR DYNAMICS STUDY OF ELECTROMIGRATION

SRI International

Herbert F. Helbig



APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

Rome Laboratory
Air Force Materiel Command
Griffiss Air Force Base, New York

This report has been reviewed by the Rome Laboratory Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS it will be releasable to the general public, including foreign nations.

RL-TR-94-210 has been reviewed and is approved for publication.

APPROVED: Joseph V. Beasock

JOSEPH V. BEASOCK
Project Engineer

FOR THE COMMANDER: John J. Bart

JOHN J. BART
Chief Scientist, Reliability Sciences
Electromagnetics & Reliability Directorate

If your address has changed or if you wish to be removed from the Rome Laboratory mailing list, or if the addressee is no longer employed by your organization, please notify RL (ERDR) Griffiss AFB NY 13441. This will assist us in maintaining a current mailing list.

Do not return copies of this report unless contractual obligations or notices on a specific document require that it be returned.

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	November 1994	Final Jul 93 - Dec 94

4. TITLE AND SUBTITLE
MOLECULAR DYNAMICS STUDY OF ELECTROMIGRATION

5. FUNDING NUMBERS
C - F30602-91-D-0001,
Task N-3-5733
PE - N/A
PR - 2306
TA - F4
WU - P6

6. AUTHOR(S)
Herbert F. Helbig

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
SRI International
333 Ravenswood Ave
Menlo Park CA 94025

8. PERFORMING ORGANIZATION REPORT NUMBER
N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Rome Laboratory (ERDR)
525 Brooks Road
Griffiss AFB NY 13441-4505

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
RL-TR-94-210

11. SUPPLEMENTARY NOTES
Rome Laboratory Project Engineer: Joseph V. Beasock/ERDR/(315) 330-4029

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

A software package has been assembled (written and adapted from commercial sources) that allows three dimensional atomic level modeling, simulation and visualization of polycrystalline samples subjected to various stresses. Sample preparation, is accomplished with a commercial software package, ADESH, that allows initial atomic coordinates to be prepared conveniently for submission to the dynamics portion of the code. The code, mdem.exe, that traces the atom motions was written in the C programming language for convenient portability across computing platforms. On an Intel 486/66 class machine, it can provide 10 ps of history for a system containing 1896 atoms in approximately 62 hours of computing time. Temperature control is provided by a thermostat function known to preserve the statistical integrity of the dynamic variables. Several techniques have been developed for visualization of the output data. Preliminary results demonstrating thermal expansion, specific heat, self-diffusion and annealing behavior have been published.

14. SUBJECT TERMS	15. NUMBER OF PAGES
Molecular dynamics, electromigration, mass transport	28
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

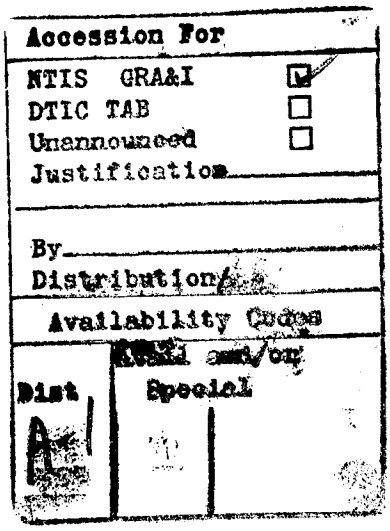
EVALUATION

Electromigration (the transport of metal atoms along a metal conductor due to high current stress and resulting in voids and eventual opening of the conductive path) is a major impediment to the miniaturization of microcircuits. Electromigration resistance is dependent on the microstructure of the metallization. Unfortunately, most of the information available on microstructure is of a qualitative nature. New techniques are needed for studying microstructure at the atomic level to determine if unique structure exist at sites where vacancies collect to form voids.

To this end a software package has been assembled that allows three dimensional atomic level modeling, simulation and visualization of polycrystalline samples subjected to various stresses. Preliminary results demonstrate reasonable values for thermal expansion, specific heat, self-diffusion and annealing behavior of aluminum films. This software will be invaluable in our investigation of diffusion related phenomena that cause degradation and failure of military and commercial microcircuit devices.

Joseph V Beasock

Joseph V Beasock
Project Engineer



ABSTRACT

A software package has been assembled (written and adapted from commercial sources) that allows three dimensional atomic level modeling, simulation and visualization of polycrystalline samples subjected to various stresses. Sample preparation, is accomplished with a commercial software package, ADESH, that allows initial atomic coordinates to be prepared conveniently for submission to the dynamics portion of the code. The code, `mdem.exe`, that traces the atom motions was written in the C programming language for convenient portability across computing platforms. On an Intel 486/66 class machine, it can provide 10 ps of history for a system containing 1896 atoms in approximately 62 hours of computing time. Temperature control is provided by a thermostat function known to preserve the statistical integrity of the dynamic variables. Several techniques have been developed for visualization of the output data. Preliminary results demonstrating thermal expansion, specific heat, self-diffusion and annealing behavior have been published.

Task Status

As the attached Man-loading Summary shows, 1544 of the 1600 hours contracted for Dr. Helbig's time under Subcontract CB0315 were completed by the end of the contract term. Mr. Bartelt completed 760 of the 800 hours that had been proposed. Thus, of the anticipated 2400 man hours, 2304 or 96% were completed and billed. The difference between the actual and anticipated hours is due primarily to the fact that Professor Helbig was hired as a full-time employee of Rome Lab approximately 90 calendar days before the scheduled contract completion date. With the submission of this report, the work of Subcontract CB0315 is concluded.

Summary of Work Completed

Although we did not complete all the work we had hoped to, virtually all of the tasks specified in the Statement of Work were completed. The chief disappointment resulted from an overly optimistic assessment of the "electron wind" problem. This final report takes as its six Section headings the six sentences of the Statement of Work, and describes how each of the specified tasks was accomplished.

1. OVERVIEW

> "***The purpose of this effort is to develop atomic level modeling and simulation software that characterizes metallization stripes and their resistance to mass transport.***"

From the outset, it was clear that computing power will not be available in the near term to simulate anything approaching a complete metallization stripe. The best current fabrication technology cannot

deliver a workable stripe with a volume significantly less than 1 cubic micron containing about 10^{12} atoms. The best current computer technology can, in practical times, handle computations involving perhaps 10^6 atoms. Wording later in the Statement of Work (Section 2.) makes it clear that subunits of a stripe, consisting of a few crystalline grains, are the systems of interest in this work. In particular, the interfaces or grain boundaries between two such crystallites appear to be the most likely routes for mass transport inside a metallic system.

At the conclusion of the project, a software package has been assembled (written and adapted from commercial sources) that allows three dimensional atomic level modeling, simulation and visualization of polycrystalline samples subjected to various stresses. Sample preparation and visualization are handled by commercially available programs as described in Sections 2. and 6. below.

The program `mdem.exe`, compiled from its C-language source-code modules, was written to follow efficiently the motions of assemblages of atoms presented to it as a file listing their phase space coordinates (positions and velocities) at some instant and species identifiers. The program reports its results in the form of files that record a) the system temperature versus time and b) the system phase space coordinates versus time. The output files containing phase space coordinates are in the same format as the input file making it convenient to chain data collection runs together.

This software has been tested and debugged on a several model systems. Results for a single crystal sample of 43 atoms and a bi-crystal sample of 601 atoms have been published[1]. During the final weeks of the contract, a bi-crystal containing 1896 atoms with an oblique grain boundary was studied. Both the 601-atom and 1896-atom bi-crystal samples were subjected to thermal and mechanical stresses that resulted in the transport of atoms to locations significantly removed from their original locations. These atomic motions were, however, minority events; the vast majority of atoms displayed a remarkable tendency to retain the crystalline structure with which they were originally endowed.

It should be noted that for both of these bi-crystal experiments, no external constraints were imposed on the samples that would have artificially maintained the integrity of their crystal structure. Nevertheless, the crystal structure *was* retained locally (with small perturbations) by the simple (Lennard-Jones) force model used. The accumulation of small perturbations to the perfect crystal structure resulted in long range distortions such as twisting and bending. These effects are evident from a comparison of Figures 1. and 2. which show orthographic projections of the initial configuration of the 601-atom sample and its condition after it had stabilized at 123 K. The atom layers were initially arrayed in planes parallel with the x-y plane. The grain boundary was essentially coincident with the plane $x = 0$. The evident twisting and bending are due to a large initial attractive force between the two crystalline components, to the misalignment of their crystal axes, and to the asymmetry of the two crystallites; that on the left contains fewer atoms and is missing most of its $z = 0$ plane. The lone atom on the left was ejected by the shock wave produced by the collision of the two crystallites and then captured as an adsorbed particle.

2. SAMPLE PREPARATION

"Acceptable software shall include tools for constructing thin film metallization consisting of a minimum of three grains that accurately simulates microelectronic metallization microstructure in three dimensions."

As indicated in Section 1., the strategy that evolved to create the simulation package called for in the Statement of Work was to separate the three constituent tasks; 1) constructing suitable arrays of initial atomic coordinates, 2) following the motions of the atoms as they moved from their initial positions, and 3) analyzing the results.

The first task amounts to sample preparation, and is chiefly a geometric one; modeling in the sense of molding or sculpting the atoms into sensible arrangements to simulate portions of a polycrystalline solid. Two complete solutions to the sample preparation problem were found in the course of the work. A working sketch called MAKECRYS.BAS was constructed in QuickBasic, and with it the 601 atom bicrystal was prepared for dynamic study. Much of this sketch was reduced to C-code, but development was deferred while the second task, that of the particle dynamics, was solved. Our expectations that this would provide us with a better understanding of the overall problem were fulfilled. Before we returned to the sample preparation problem, a commercial software package, (ADESH© from CASA) was identified that allows initial atomic coordinates to be prepared conveniently for submission to the dynamics portion of the code.

The 1896-atom bi-crystal mentioned in Section 1. was created by ADESH. It is shown in near-orthographic projection in Figure 3. Figure 4. shows the same system after annealing at 10 K. Further discussion of this system appears in Section 4.

It is not difficult to generate the coordinates of atoms that represent a crystallite of desired lattice constant and orientation. One merely defines a suitably positioned and oriented set of basis vectors, and then systematically multiplies them by integers. If the crystal requires more than one atom per unit cell, that presents only small complication; a set of basis vectors internal to the unit cell must be defined, and used to add the appropriate additional atoms to each unit cell.

The chief difficulty lies in terminating the list of atomic coordinates so that they lie within some desired geometric bounds. In the QuickBasic sketch mentioned above, we provided for crystallites bounded by convex, but otherwise arbitrary polyhedrons with up to twenty faces, each face containing up to ten edges. Within each polyhedron the user could specify the coordinates of one atom, and a set of basis vectors to fix the crystal orientation and lattice constant. The program then filled the polyhedron by systematically adding atoms coordinates and checking for each new trial coordinate set that it was inside the bounding polyhedron. The search for additional coordinates was continued out to a rectangular parallelepiped, defined by the basis vectors, that circumscribed the desired polyhedron.

The ADESH code presumably goes through a similar process to generate sets of atomic coordinates, but the authors simplified their task by restricting the bounding solids to rectangular parallelepipeds, or segments (including the full figure) of a cylinder or sphere. Although this seemed at first to be restrictive, we were able to construct a bicrystal sample that included a grain boundary oblique to the bounding surfaces as Figure 3. illustrates. We have not, in fact, found ways to construct crystallites using ADESH that would combine to form a truly three dimensional triple point joining three crystallites. If CASA, Inc. or another commercial vendor does not provide a solution to this problem, it will be necessary to complete the development of MAKECRYS.BAS into C-code.

3. PHYSICAL CONSTANTS

> ***"The software shall be capable of determining accurate physical constants for the material being modeled, such as Young's modulus, thermal coefficient of expansion, thermal conductivity, diffusion coefficients, etc."***

Our treatment of physical constants proceeded in this way. The two free parameters in the Lennard-Jones potential function, which was used to model the atomic interactions, were chosen to reproduce the known lattice parameter and Young's modulus for aluminum.

The resulting thermal coefficient of expansion, α, was then determined for a 43-atom spherical cluster from the slope of the fractional change of its average maximum dimension versus its temperature. The value of α obtained in this way was larger than measured values for aluminum by a factor of about 20. This was attributed to the fact that the Lennard-Jones binding energy was modeled on the engineering value of Young's modulus for Al, not on the larger value that would pertain to an ideal crystal. Had the larger value been used, α would have been in closer accord with measurement. It is pertinent that the ADESH program mentioned above uses a Lennard-Jones binding energy for Al that is eight times larger than that used in our work. Their value is in accord with the heat of formation of aluminum.

At best, however, the Lennard-Jones potential has not proven very effective as a model of metallic bonding, and no significant time was spent exploring the details of this potential model. The simulation code will easily accept alternative potential functions; we are looking forward to implementing more sophisticated interaction models.

The self-diffusion coefficient for Al was also determined. This was done for the 601-atom bi-crystal by recording the mean-square displacement of its atoms after it had reached a stable mean kinetic energy corresponding to a temperature of 123 K. Not surprisingly for this temperature, the self-diffusion coefficient was found, within the error imposed by thermal fluctuations for such a small system, to be zero. This result is consistent with the stability of the system that was observed using a variety of visualization techniques. Experiments at higher temperatures and with the presence of

vacancies have not yet been made, but the capability of doing so has been demonstrated.

A third physical constant was determined, namely the specific heat of the 43-atom cluster mentioned above. The expected value for a system constrained by the laws of classical mechanics is that of Dulong and Petit, and, within the uncertainty of thermal fluctuations, that was the value found.

No measurements have yet been made of thermal conductivity, but the thermostat function contained in the simulation could easily be set to different values at opposite ends of a sample and monitored for the time averaged injection (at the hot end) and extraction (at the cold end) of energy. These, together with the sample dimensions provide the necessary data to compute the thermal conductivity.

4. MECHANICAL, THERMAL, ELECTRICAL STRESSES

> ***"The software shall provide introducing stress, temperature, and thermal and electrical gradients into the simulated metallization stripe."***

Mechanical stress can be introduced into the simulated atomic system either statically or dynamically. Static stress may be introduced by fixing the positions of atoms at opposite ends of the sample in such a way that they cannot all be part of a perfect crystal. If, for example, the entire collection of surface atoms is fixed, the interior regions will be subjected to either positive or negative pressures depending on the temperature of the system. Similarly, atoms on opposite faces can be fixed in such a way that sheer, torsional, compressive or tensile stresses (or combinations of them) are imposed. Although this facility is present, no experiments have yet been conducted employing static mechanical stresses.

Dynamic mechanical stress is necessarily imposed when a system is prepared in a non-equilibrium configuration, and then allowed to relax via molecular dynamics simulation. Since it is virtually impossible to select the initial phase space coordinates for a system of any complexity so that it will be in an equilibrium configuration, such dynamic stresses are unavoidable. They can be minimized, for example, by utilizing a non-dynamic technique to relax the system before beginning molecular dynamics simulation. The ADESH program uses Monte Carlo methods to do just this.

Alternatively, one can rely on a thermostat function to cushion the effects of initial, non-equilibrium conditions. This is successful provided the initial conditions are reasonably close to equilibrium. The warped condition of the 601-atom sample pictured in Figure 2 and its having annealed from a bicrystal with a grain boundary to an imperfect single crystal is due in large part to dynamical stresses that developed as the two crystallites collided. The temperature record of this encounter is shown in Figure 5. When the same system was allowed to relax with a thermostat function active and set at 1 K, the peak temperature reached was 3.5 K, and thereafter the system temperature settled down within 10 ps to acceptably small fluctuations about 1 K as shown in Figure 6. Importantly, the grain boundary was preserved, so that this system can now serve as the starting point for studies of mass

transport along (and perpendicular to) a grain boundary with at least some thermodynamic stability. Whether that stability will survive heating to interestingly high temperatures, let alone electromigration stresses, remains to be seen.

Several experiments of this nature were conducted, and it was found that the thermostat function can become unstable if one attempts to change the system temperature too rapidly. With 2 fs integration time steps, temperature changes as large as 10 K are successful. Figure 7. shows the well-behaved temperature evolution of the 1896-atom bicrystal as it evolved from rest (0 K) as shown in Figure 3. for a time interval of 10 ps. Figure 4. shows its final configuration at 10 K. For larger temperature changes, the system mean kinetic energy will fluctuate with large and often catastrophic amplitude. Figure 8. shows the result of attempting to raise the temperature of the 1896-atom sample from 10 K to 100 K. Clearly, the thermostat was unable to cope with this large temperature change using the same integration time-step and time constant as were used to obtain the result shown in Figure 7.

From the foregoing discussion, it is apparent that temperature control is provided for in the simulation code. We have implemented the Nosé-Hoover[2] thermostat function as described by Valkealahti and Manninen[3] to accomplish this. Although no experiments have yet been done with thermal gradients, by setting the temperatures of different groups of atoms to different temperatures, such gradients can easily be created and studied as mentioned in Section 3 in the discussion of thermal conductivity.

Electric fields (i.e., voltage gradients) can easily be introduced as additions to the force function that operates on each atom in the function `move_atoms` in the C-code module `mdemutil.c`. A uniform electric field acting on an atom (considered as a positive ion due to its sharing of non-localized electrons with the crystal) would be represented as a constant additional force *parallel* with the direction of the electric field. A variation of this notion is, in fact, a standard procedure in continuum models of electromigration where the lattice ions are endowed with an effective charge, Z^*, taken to *negative* in order that the atoms should move (in accordance with observation) *anti-parallel* with the electric field (in the direction of the electron motion). In our view, this ploy to attribute the ion motion *directly* to the electric field, rather than to the action of electrons as the *agents* of the electric field, is unwarranted in a model intended to reflect as accurately as possible all of the influences at work at the atomic scale.

Unfortunately, we have not yet been able to introduce a satisfactory model of electron-ion interaction (energy and momentum transfer) into the simulation. Indeed, to our knowledge, no one has achieved this. As mentioned in our 4th quarterly report, a standard reference in the field, Ziman's "*Electrons and Phonons*", declares

> "Let it be said, at once, that there is no rigorous theory of the transport coefficients. The relationship between the electric current and the electric field in a metal at a fixed temperature has never been formally deduced from the equations of motion of the electrons, classical or quantal."

We are, nonetheless, trying to construct an electron-ion interaction model that will provide a

consistent picture of momentum transfer from the electrons to the ions (the "electron wind") and of excess energy transfer from the electrons to the ions (I^2R, or Joule heating). Our current thinking on this subject centers on the following notions. Electrons and ions in a conductor are constantly exchanging energy as a result of collision processes. At thermal equilibrium, and in the absence of an electric current, the transfer of energy from the electrons to the lattice and to the electrons from the lattice must proceed at nearly identical rates. The difference appears to be I^2R heating of the lattice by thermally driven current fluctuations (Johnson noise). One might suppose that this excess energy delivered to the lattice escapes from the conductor radiatively. For this picture to be consistent, the cooling of the electrons due to Johnson noise must be offset by the energy absorption processes that maintain the conductor in thermal equilibrium with its environment, e.g., the absorption of radiation from that environment. These are the background activities upon which is superposed the tiny electron drift that constitutes even a large DC current (i.e., the electron wind). A model of electron-ion interactions that accounts for these processes is what we are presently seeking.

5. PROGRAMMING LANGUAGE

> "*The source code shall be delivered to Rome Laboratory for future development, shall be written in the ANSII Standard Version of the C programming language, and shall build upon software previously developed at Rome Laboratory.*"

The simulation software generated under this contract is an outgrowth of software developed at Rome Lab during the Summer of 1993. It has been delivered to Rome Laboratory and is under continuing development in the very real sense that the principal investigator is now a full-time employee of the Lab and is devoting most of his effort to improving and extending the software.

The executable program, `mdem.exe`, that follows the motions of the atoms comprising the sample system was compiled from four modules written in the ANSII Standard C programming language. The latest version of the code was compiled as 32-bit DOS code to run on a 486-class personal computer. The compiler chosen for this work was the WATCOM C/C++ compiler (version 10). It has the capability to compile and optimize the same source code for other operating systems including OS-2 and Windows NT. Compilation for UNIX based machines should pose no problem because the WATCOM integrated development environment will screen the source code for ANSII standardization.

The four modules are `mdem.c`, `mdemio.c`, `mdemutil.c`, and `mdemmem.c`. They are accompanied by so-called "header files" of the same name but with the extension `.h` that contain declarations of external variables and functions from the standard library.

The module `mdem.c` contains the function named "`main`" that the C-compiler treats as the control module. It accepts command-line arguments that determine the data file in which the phase space coordinates are to be found, the number of integration steps to be made (`nsteps`), the integration

time-step, the thermostat function initial value, the desired system temperature and the number of integration steps between the output of phase space files. Its chief function is to execute a loop in which it calls the function `move_atoms` `nsteps` times. It also keeps track of elapsed time, moves array pointers, integrates the thermostat function, check for user interrupts, writes useful status information to the screen and writes data files to disk within this loop. Prior to entering the loop, it calls functions from the other three modules to perform various initializations, and after the loop terminates, it closes the program in an orderly fashion.

The module `mdemio.c` contains input/output functions used by `mdem.c` to read various sorts of data from the initial data file, to acquire date/time information from the operating system (for use in naming output files) and to write the phase space coordinates to disk.

The important content of the module `mdemutil.c` is the function `move_atoms`. It performs the numerical integrations whereby each atom is moved in accord with its current phase space coordinates (position and momentum), the forces exerted on it by all the other atoms within its sphere of influence and the force that the thermostat function imposes to control the temperature. This module also contains functions to compute the system kinetic and potential energies, and some incidental functions dealing with the system linear and angular momentum (that are presently unused).

The module `mdemmem.c` contains functions that allocate and de-allocate memory for various scalar, vector and tensor quantities. Some of these are currently unused. The data structure of primary importance is the collection of phase space coordinates and a parallel array containing the tags that identify the species of each atom. Currently, only collections of identical atoms have been studied, but the tag array provides for differing interactions among several species.

6. VISUALIZATION

> *"A graphical interface for constructing the model and interpreting the output shall also be considered."*

Several means were explored to provide visualization of the data that were collected from the simulated experiments described in the previous sections. Figures 1. through 4. exemplify the most satisfactory two-dimensional graphical presentations of the atomic configurations studied. They were prepared using the commercial data analysis program Origin from Microcal, Inc. Origin is also capable of displaying atomic configurations as two-dimensional projections (true perspective or orthographic) of their three-dimensional positions. As a pertinent example, Figure 9. is a perspective projection of the 1896-atom sample in its final, 10 K condition.

In addition to Origin, code was written in QuickBasic to produce three-dimensional perspective views of the samples, and the commercial package SigmaPlot from Jandel, Inc. was evaluated. The

drawback with QuickBasic is that it is restricted to VGA (640 X 480 pixels) graphics. This is unacceptable compared with the 1024 X 768 graphics now generally available even on PC-class computers. SigmaPlot was rejected because it cannot render a three-dimensional view of two sets of differently colored (or shaded) objects that properly preserves the "back-to-front" order of all objects. The result is that objects which should be hidden by others closer to the viewpoint, are not.

Finally, a cinematic presentation was prepared of the evolution of the 601-atom system from its initial condition (Figure 1.) to its final condition (Figure 2.) by placing 95 intermediate position plots (like those of Figures 1. and 2.) successively on the video screen. In the interests of a smooth visual effect, the previous plots were not erased, so the effect was to see the paths of the 601 atoms develop simultaneously. By watching this video presentation closely and repetitively, it was possible to detect the three surges of kinetic energy that are visible in the temperature record of Figure 5; the initial impact of the two crystallites is followed by three cycles of a bending-mode oscillation before thermalization sets in.

This code was written in QuickBasic. The VGA graphics limitation was tolerable for this application which represented each atom position as a single pixel. The projected atom positions were reduced to integer representation to allow maximum speed of data handling and to maximize the number of points that could be held in RAM.

Attachments:

1) Man-loading Summary

2) 4th Annual IEEE Dual-Use Technologies & Applications Conference, Vol. II, pp. 98-101

References:

1. *Progress Toward a Molecular Dynamics Simulation of Electromigration,* H.F. Helbig, T. Bartelt, L.H. Walsh and J.V. Beasock, 4th Annual IEEE Dual-Use Technologies & Applications Conference Proceedings, Vol. II, May, 1994.

2. W.G. Hoover, Phys. Rev. A **31** (1985) 1695.

3. S. Valkealahti and M. Manninen, Computational Materials Science **1** (1993) 123.

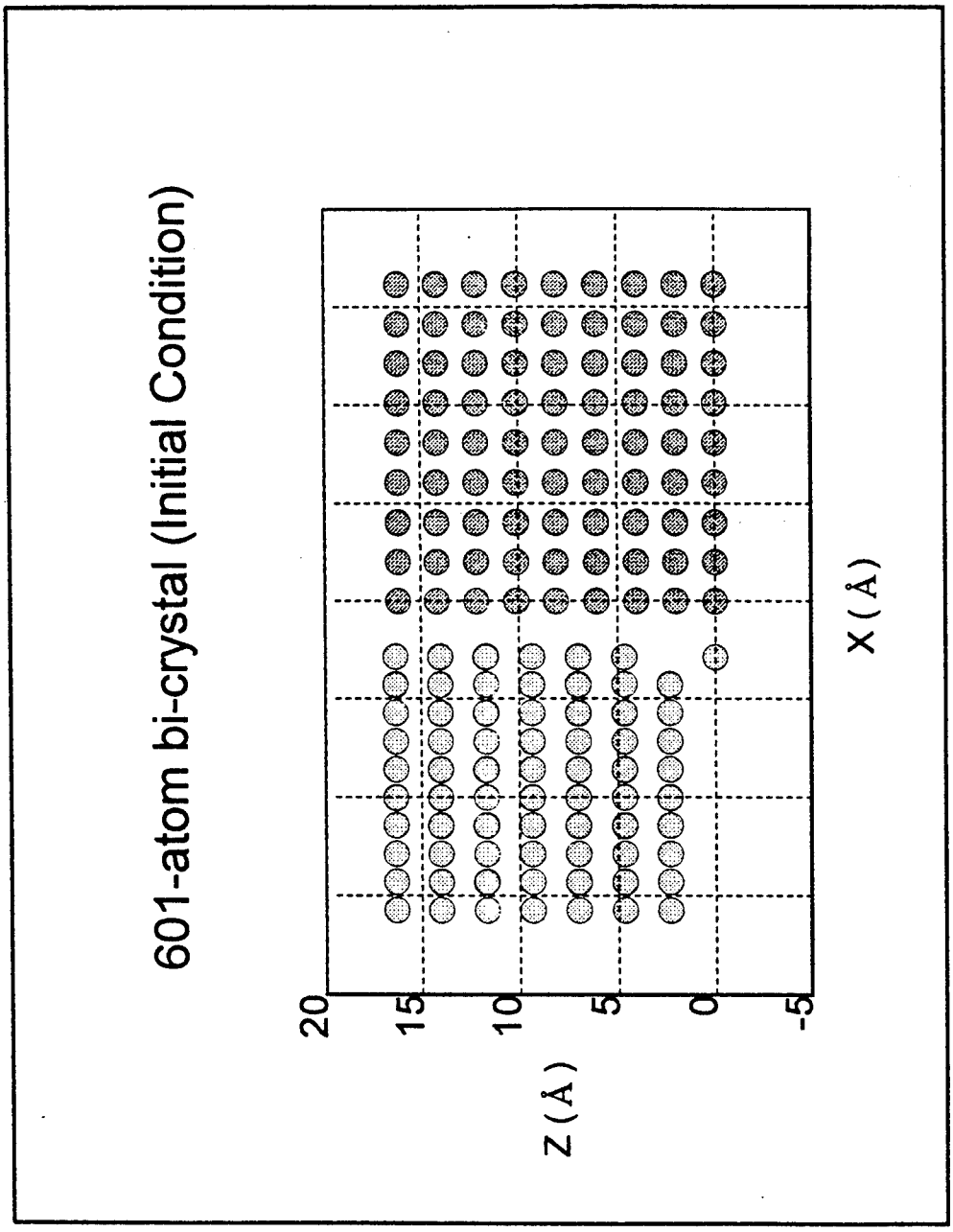


Figure 1 Simulated Al bi-crystal at rest (0 K).

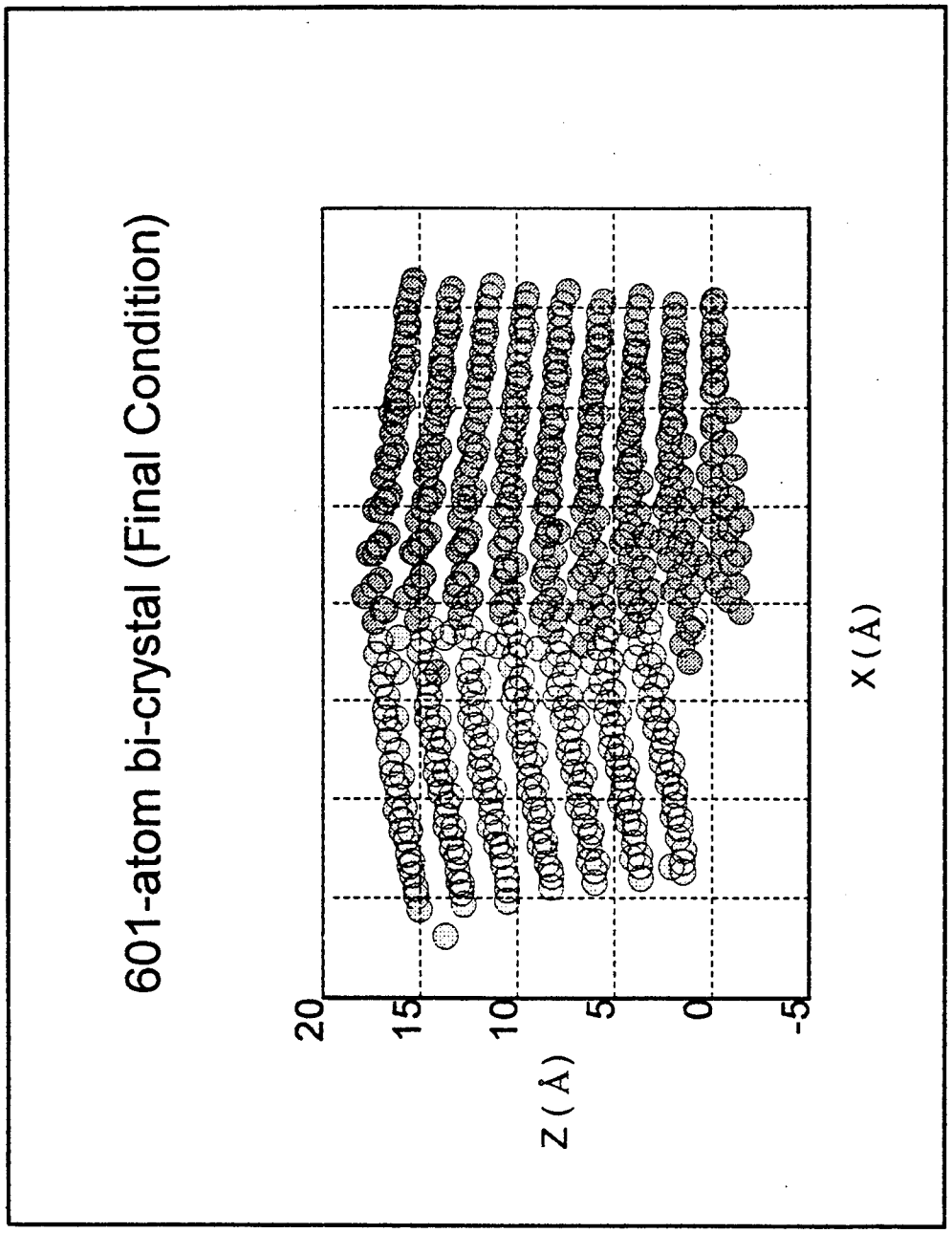


Figure 2. Simulated Al crystallite, after 12 ps (123 K).

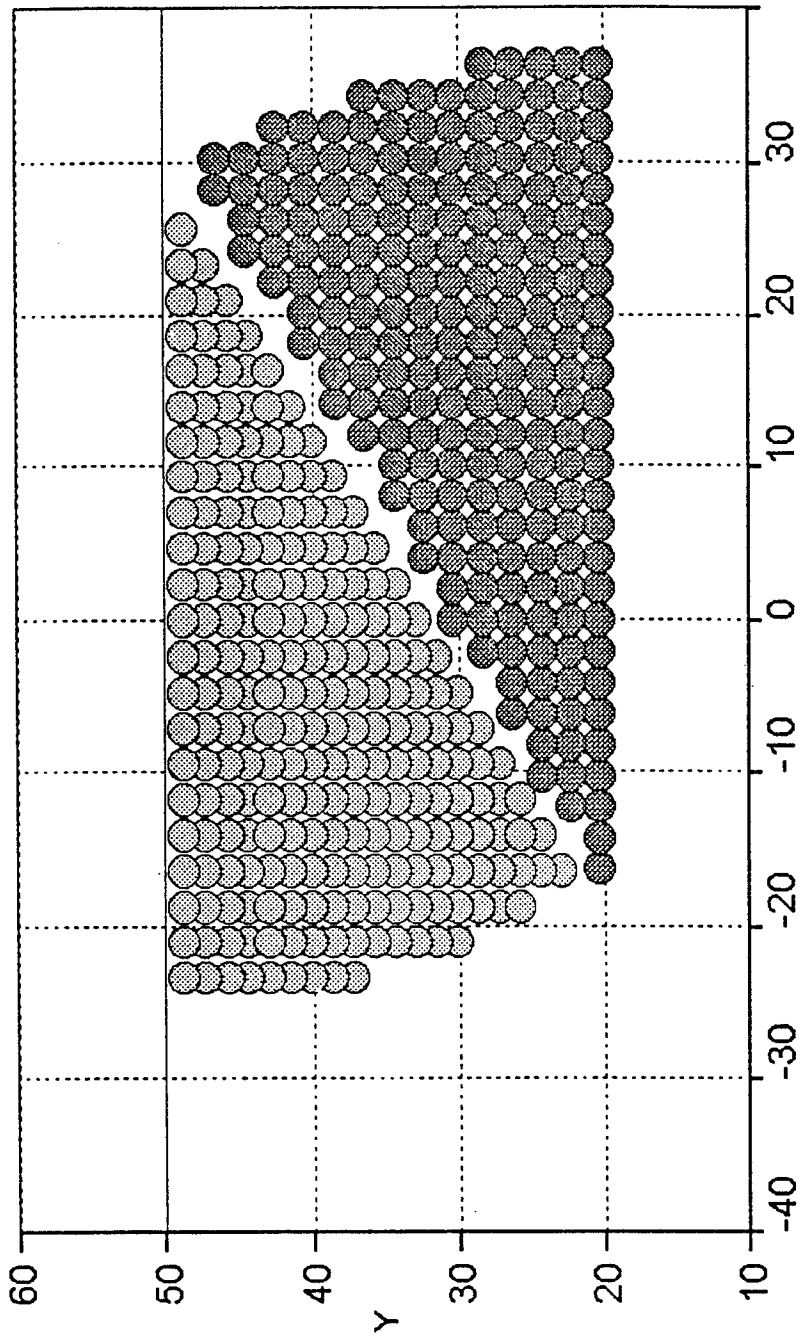


Figure 3. 1896-atom bi-crystal from ADESH (Initial Condition)

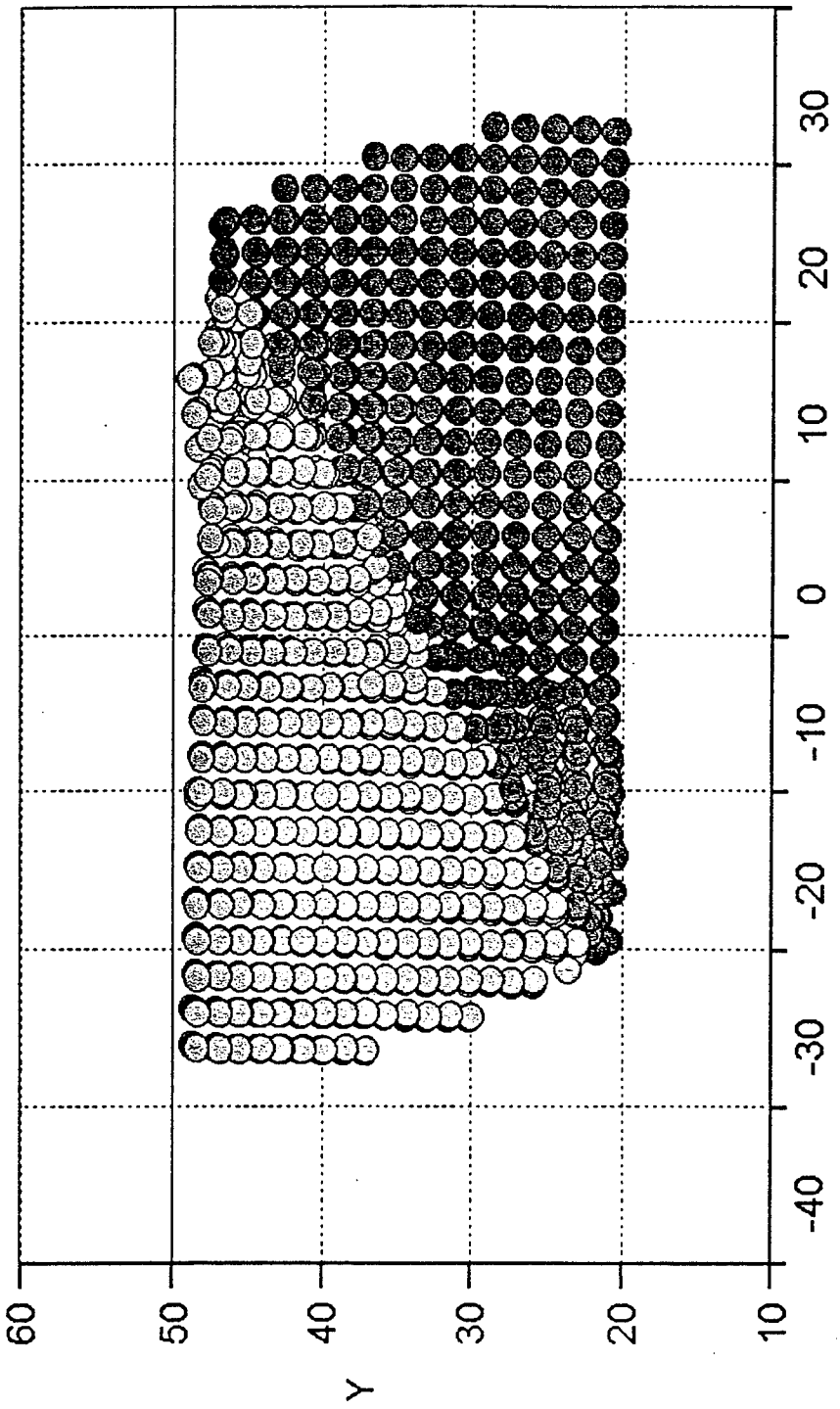


Figure 4. 1896-atom bi-crystal (10 K)

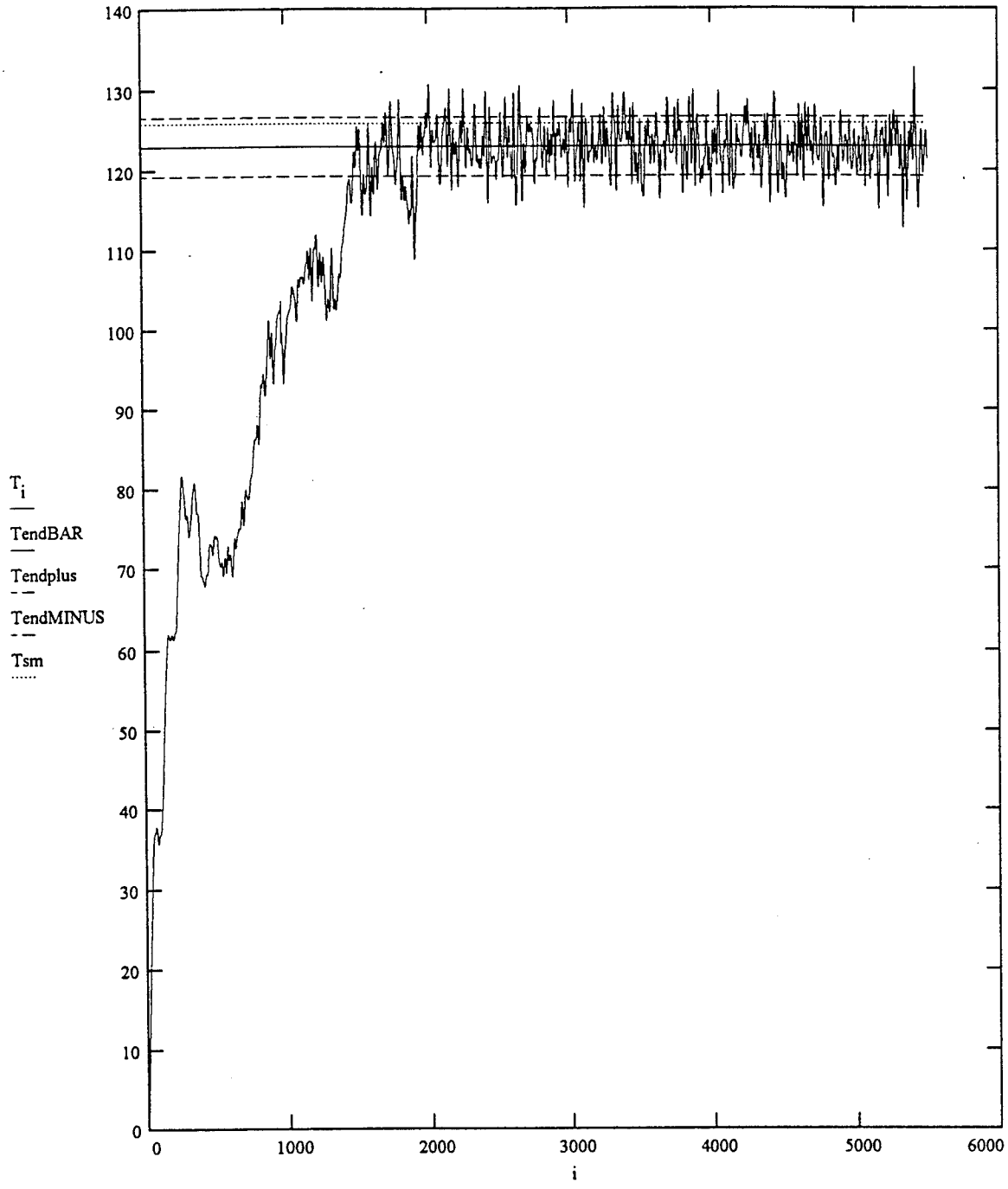


Figure 5 Temperature vs. Time for 601 atom bi-crystal. Auxilliary lines show mean temperature, rms fluctuation and stat. mech. expected fluctuation. Total time ~ 13 ps.

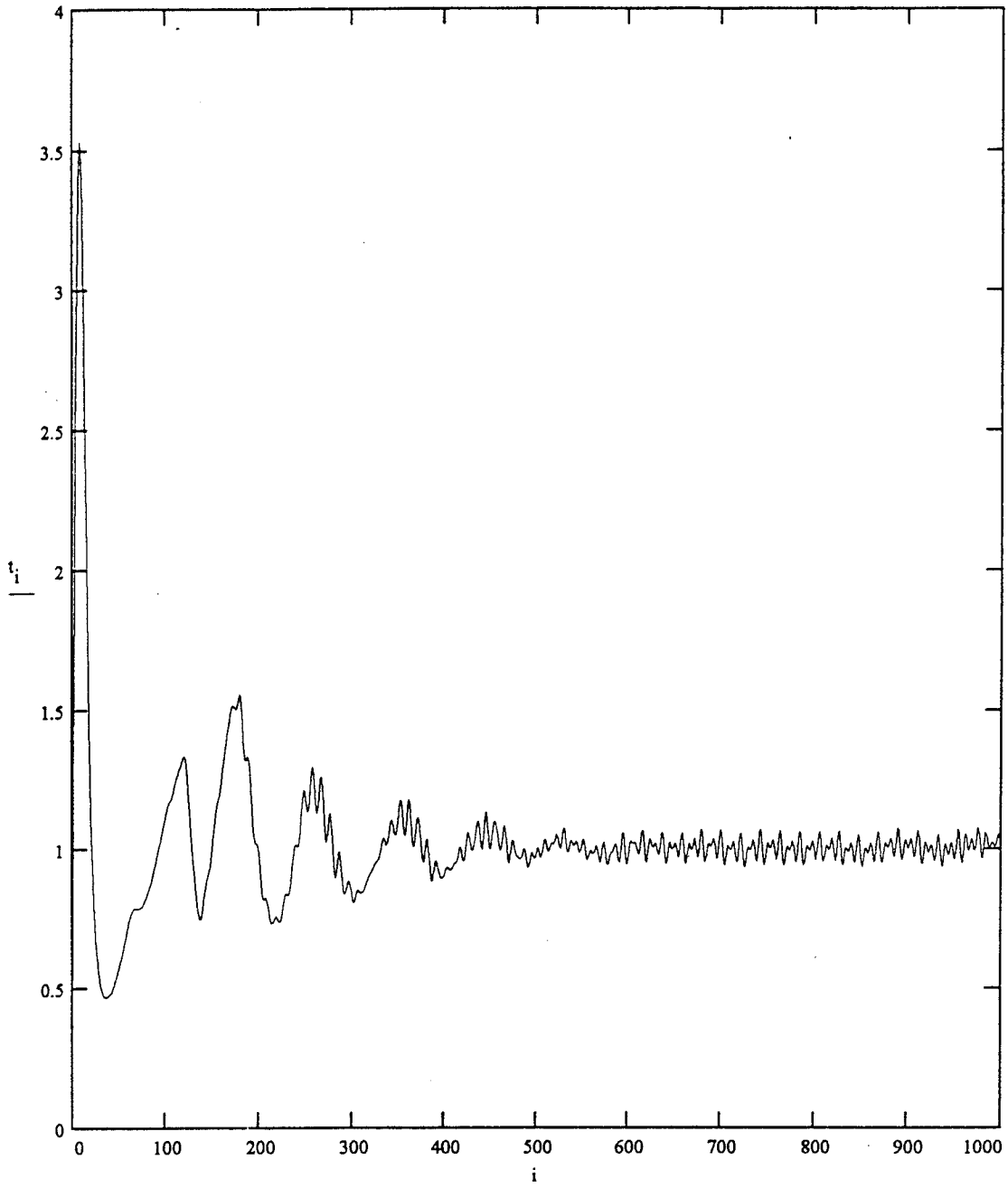


Figure 6 Temperature versus time for the 601-atom system with the thermostat function active and set to 1 K.

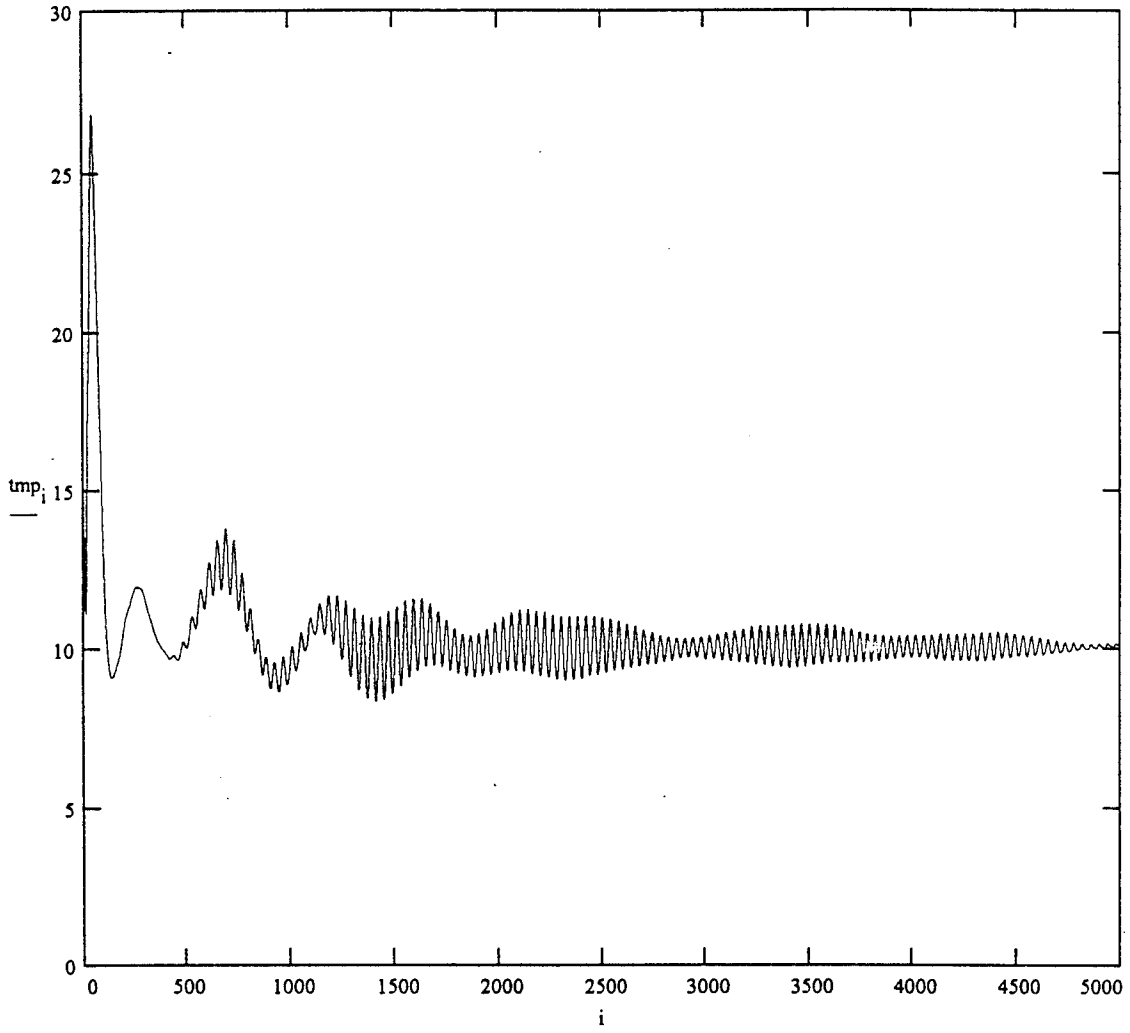


Figure 7 Temperature versus time for 1896-atom bicrystal starting from 0 K and with thermostat set at 10 K.

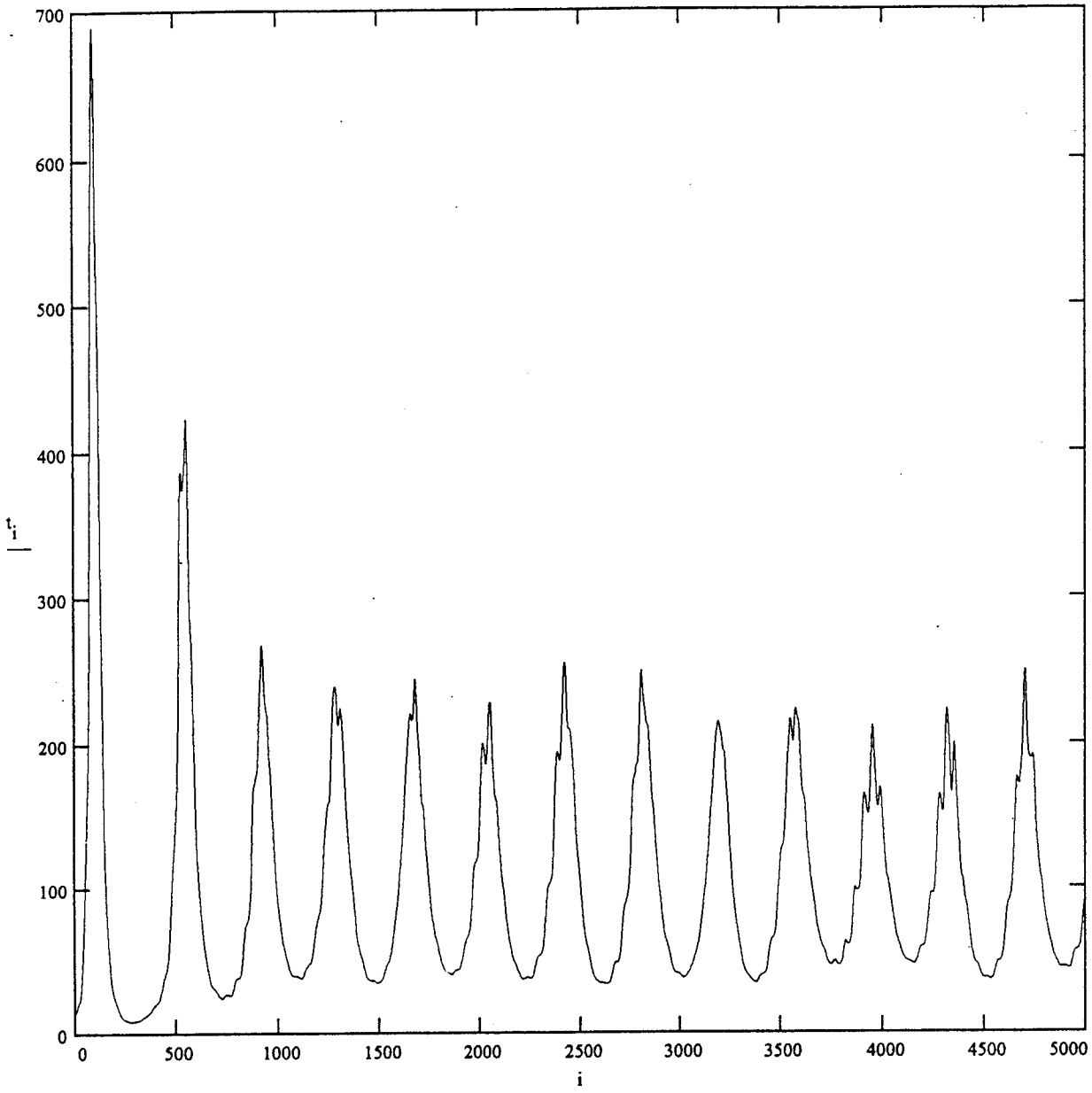


Figure 8 Temperature versus time for 1896-atom bi-crystal starting from 10 K and with thermostat set at 100 K.

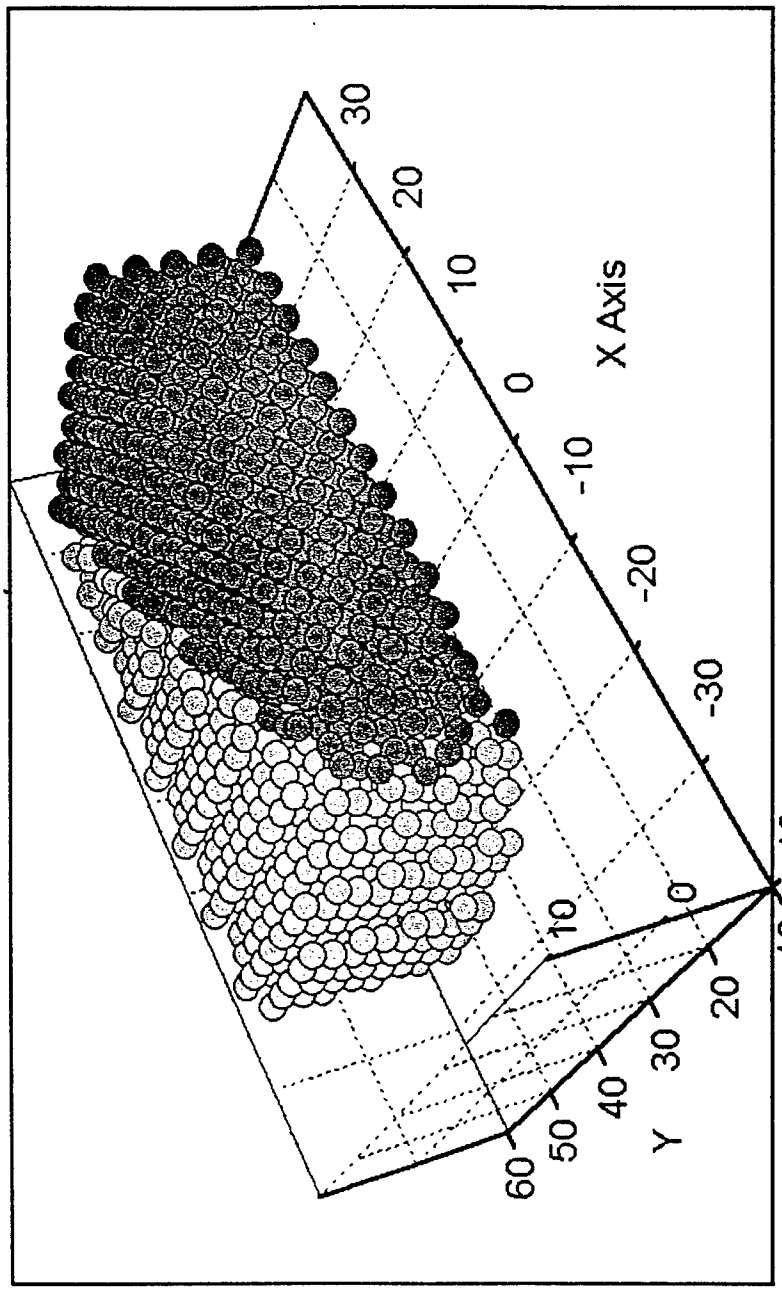


Figure 9. 1896-atom bi-crystal (10 K)

MISSION

OF

ROME LABORATORY

Mission. The mission of Rome Laboratory is to advance the science and technologies of command, control, communications and intelligence and to transition them into systems to meet customer needs. To achieve this, Rome Lab:

a. Conducts vigorous research, development and test programs in all applicable technologies;

b. Transitions technology to current and future systems to improve operational capability, readiness, and supportability;

c. Provides a full range of technical support to Air Force Materiel Command product centers and other Air Force organizations;

d. Promotes transfer of technology to the private sector;

e. Maintains leading edge technological expertise in the areas of surveillance, communications, command and control, intelligence, reliability science, electro-magnetic technology, photonics, signal processing, and computational science.

The thrust areas of technical competence include: Surveillance, Communications, Command and Control, Intelligence, Signal Processing, Computer Science and Technology, Electromagnetic Technology, Photonics and Reliability Sciences.