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A STUDY OF THE LIQUID-SOLID  
 INTERFACE DURING RAPID  
 RESOLIDIFICATION OF COPPER-  
 TITANIUM USING MOLECULAR DYNAMICS

THESIS

Craig L. Loisel, B.S.N.E  
 Captain, USAF

AFIT/GNE/ENP/91M-4

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Presented to the Faculty of the School of Engineering  
of the Air Force Institute of Technology  
Air University  
In Partial Fulfillment of the  
Requirements for the Degree of  
Master of Science

Craig L. Loisel, B.S.N.E.  
Captain, USAF

March 1991

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## Table of Contents

Acknowledgements .....	ii
List of Figures .....	iv
List of Tables .....	v
Abstract .....	vi
Introduction .....	1
Previous Studies .....	2
Outline .....	6
Method .....	8
Atomistic Simulation (Sabochnik, undated) .....	8
Crystal Studied .....	14
Analysis Methods .....	16
Procedure .....	23
Overview .....	23
Liquid-Solid Interface Creation .....	23
Resolidification Using Molecular Dynamics .....	24
Analysis of 773 K Runs .....	33
Estimate of Interface Velocity Limit .....	33
Trajectory and Projection Plots, 773 K .....	34
Atomic Density Plots .....	35
Interface Location Using Order Parameter .....	37
Conclusion .....	40
Appendix A: Comparison of Analysis Techniques .....	42
Bibliography .....	45
Vita .....	46

## Table of Figures

CuTi Crystal .....	15
Sample Trajectory Plot .....	17
Sample Projection Plot .....	19
Trajectories, 32-36 psec, 1000 K .....	28
MSD vs Time, T = 800 K .....	29
Crystal at 0 ps, T = 773 K .....	30
Crystal after 80 ps at 773 K .....	30
Crystal after 160 ps at 773 K .....	31
Trajectory Plot, t = 0-16 ps, T = 773 K .....	31
Trajectory Plot, t = 90-96 ps, T = 773 K .....	32
Trajectory Plot, t = 144-160 ps, T = 773 K .....	32
Atomic Density at t = 0 ps, T = 773 K .....	36
Atomic Density at t = 160 ps, 773 K .....	36
Interface Position vs Time, 773 K .....	38
Atom Positions at 80 ps, 773 K .....	43
Trajectory Plot, t = 80-96 ps, T = 773 K .....	43
Atom Density at t = 80 ps, T = 773 K .....	44

Table of Tables

Interface Velocity Limit, 1000 K .....	34
Interface Velocity Limit, 818 K .....	34
Order Parameters after 80 ps, T = 773 K .....	44

Abstract

The behavior of the liquid-solid interface during resolidification of a condensed copper-titanium crystal is studied by atomistic simulations. A system of 1080 atoms (540 of each type) was simulated. The interface was created using monte carlo techniques and resolidification was performed by molecular dynamics. Resolidification was attempted at temperatures of 1200 K, 1100 K, 1000 K, 900 K, 818 K and 773 K. The liquid-solid interface was found to move only at 773 K, resulting in a chemically disordered crystal. The interface velocity observed in the simulation is 6.6 m/s which agrees well with the theoretical value of 5.5 m/s. The low interface velocity indicates the recrystallization is governed by diffusion-limited growth.

A SIMULATION OF THE LIQUID-SOLID  
INTERFACE DURING RAPID RESOLIDIFICATION  
OF COPPER TITANIUM USING MOLECULAR DYNAMICS

Introduction

Atomistic simulation is one way to predict the results of various resolidification processes. In this study, a computer simulation is used to investigate the behavior of a liquid-solid interface during rapid resolidification of the intermetallic compound CuTi. An interface is created in a simulated CuTi crystal and then the system is held at specific temperatures for several thousand timesteps of 0.002 picoseconds each. The results from the computer simulations are examined to see if the system has resolidified and the interface moved, and if possible, calculate the interface velocity. The crystal may grow back chemically disordered, meaning that atoms occupy lattice sites but are not the same type which originally inhabited the location. The system could grow back amorphous or even undergo homogeneous freezing, forming a solid without the interface moving.

Although this appears to be a straightforward problem, all simulations and experiments performed on liquid-solid metal interfaces to date deal with single metal systems (Landman, et al, 1988a, 1988b). The simulation of these interfaces in alloys is a new region of study, with no previous work available for background. Therefore the intent of this paper is not to arrive at a specific conclusion about the interface velocity (such as determining the dependence of the velocity on temperature) nor to develop new methods of analysis or simulation, but rather to perform initial simulations of alloys and create a basis for future simulations.

#### Previous Studies

Several atomistic simulation studies on the recrystallization of metals have been accomplished, either using simulations only (Landman et al., 1988), or in conjunction with experimental studies (MacDonald et al., 1985). All the work so far has been concentrated on single metal crystals but the results from those studies are used as a yardstick or the results of this study.

MacDonald, et al., studied the crystallization of silicon, copper and gold using both experimental and computational methods. They measured interface velocities of up to 100 m/s, which supports the hypothesis pure metal recrystallization is governed by collision-limited growth.

Simply put, a crystal in the collision-limited growth regime grows quickly since any atom moving into a lattice site can fill the site with no adverse effects on the system energy. The maximum interface velocity for collision-limited growth is the speed of sound in the material

The other growth regime described by MacDonald is diffusion-limited growth, which requires a more specific rearrangement of the atoms than collision-limited growth. Diffusion-limited growth is prevalent in concentrated metallic alloys such as CuTi. As the system is supercooled the atoms will diffuse into lattice sites, thus restricting recrystallization velocity by the diffusion coefficient,  $D_L$

$$v_D \sim \lambda / \lambda^2 / D_L = D_L / \lambda \quad (1)$$

$\lambda$  is the lattice constant ( $\sim$  one interatomic distance). The diffusion coefficient for liquids is

$$D_L = \frac{MSD}{2n\Delta t} \quad (2)$$

MSD is the mean square displacement of the atoms (see Chapter III for an explanation of MSD),  $n$  is the number of degrees of freedom of the system and  $\Delta t$  is the time interval over which the MSD is calculated. For three dimensional systems,  $n = 3$ .

The velocities will initially increase with decreasing temperature because at higher temperatures the atoms have enough energy to break out of lattice sites. At some

temperature, the velocity will begin to decrease with decreasing temperatures because the atoms are moving slower and take longer to diffuse into the lattice sites. Since  $D_L \sim 10^{-5} \text{ cm}^2/\text{s}$  and  $\lambda \sim 2 \text{ \AA}$  for metals, the growth velocities in the diffusion-limited regime are on the order of 5 m/s (MacDonald et al., 1985).

Richardson and Clancy performed a simulation of resolidification of gold and copper (Richardson and Clancy, 1990). They simulated laser processing of metals by setting up a crystal-vapor interface and introducing an energy "pulse" onto the crystal surface which is at room temperature. The fluence and duration of the pulse ( $5 \text{ mJ/cm}^2$  and 20 ps) were based on the laser pulses used in the experiments by MacDonald, et al. (see previous chapter). After the "pulse" is switched off, Richardson and Clancy calculated the interface position and temperatures as functions of time.

Richardson and Clancy calculated interface velocities at three temperatures:  $0.22 T_m$  (melting temperature),  $0.53 T_m$  and  $0.92 T_m$ . Their results for copper yielded interface velocities of 82, 57 and 9 m/s respectively. They also observed some disorder in the recrystallized region at the highest temperature and contraction between the outermost crystalline layers after resolidification. The results they obtained for gold did not agree well with experimental values obtained by MacDonald et al, finding the

resolidification velocity was ~ 40 m/s. This discrepancy was probably due to deficiencies in their potential model (Richardson and Clancy, 1985: 335).

Landman et al. ran two simulations on silicon to determine the effect of growth direction on the velocity. The first (Landman et al., 1988a) simulated crystal growth on a (100) interface. They found that crystallization did not occur until the system was undercooled by 150 K and then the crystal growth proceeded at an average velocity of ~ 18 m/s. The second simulation was performed on a (111) interface (Landman et al., 1988b). Again, 150 K undercooling was required before recrystallization was observed. They employed two different cooling rates to their system. The "fast" rate simulations gave a growth velocity of ~ 14 m/s and the "slow" simulations resulted in a growth velocity of 9 m/s. The flat solid-liquid surface was maintained during the growth. The crystallization was discontinuous on the (111) surface; the crystal would experience periods of fast growth disrupted by intervals in which the interface would not move. In contrast, the (100) surface grew uninterrupted.

LCDR Charles L. Wood, USN, performed atomistic simulation of the melting point of CuTi as part of a research apprenticeship at the Air Force Institute of Technology. He used the same computer code and interatomic potentials as in this study. Wood found the simulation

yielded a melting point for CuTi of 1287 K which compared well with the experimental value of 1257 K. Although he did not study interfaces, his results indicate the potential functions used in this simulation are accurate.

The rationale for studying interfaces in metals may not be readily apparent. In laser processing of materials, the laser imparts short (pico- or nanosecond) pulses of energy into the metal, creating large temperature gradients. The surface of the metal melts and the liquid-solid interface moves deeper into the metal. When the pulse ends the heat flows into the solid substrate causing rapid cooling of the melt. The melted region becomes undercooled below the equilibrium freezing temperature, causing the interface to reverse and progress toward the surface of the metal. The kinetics of the heat flow determine the structure of the resulting solid, either crystal or amorphous (Chokappa et al., 1989). Simulations like this one will become more important as new material processing methods are developed.

### Outline

Chapter II gives a background of atomistic simulation. The information is sufficient to give a basic understanding of the mechanisms of atomistic simulation. The specific computer code used in this study is also explained, and a brief description of the crystal simulated is given. Chapter III describes in some detail the procedure used to

simulate resolidification of the CuTi. Chapter IV analyzes the results of the simulation at 773 K which yielded a recrystallizes system. Chapter V summarizes the work and states the conclusions drawn from the simulation.

## Method

### Atomistic Simulation (Sabochnik, undated)

Atomistic simulation is a method of performing computer experiments on materials based on the premise that if interactions between individual atoms are known, the motions of the atoms can be calculated, thereby simulating small systems. Atomistic simulations fall into three categories: molecular statics (MS), monte carlo (MC) and molecular dynamics (MD). Molecular statics is used to find stable energy configurations of atoms in crystals, and is not very useful in non-equilibrium studies such as this. Molecular dynamics simulates the behavior of the atoms by solving Newton's equations of motion for the system, giving the position and velocity of each atom in the system.

For atomistic simulation to work properly, the interatomic potential, which determines how the atoms interact with one another, must be known. The interatomic potential is used to calculate the total energy of the system. Oh and Johnson developed an approach to developing interatomic potentials based on the embedded-atom method (EAM) which is used in this study (Oh and Johnson, 1988). In EAM, the potential energy for a system is given by

$$U_{tot} = \sum_i F_i \left( \rho(r_i) + \sum_{j < i} \phi_{ij}(r_{ij}) \right) \quad (3)$$

$U_{tot}$  is the potential energy,  $\bar{r}_i$  is the position of atom  $i$ ,  $F_i(\rho_i)$  is the energy needed to imbed an atom  $i$  into the electron density  $\rho_i$  and  $\phi_{ij}(\bar{r}_{ij})$  is the repulsive potential between atom  $i$  and atom  $j$  separated by a distance  $r_{ij}$ . The subscripts  $k$  and  $m$  denote the species of atoms  $i$  and  $j$  respectively. The electron density,  $\rho_i$  is found by

$$\rho_{(i)} = \sum_{j \neq i} f_j(r_{ij}) \quad (4)$$

$f_j(r_{ij})$  is the contribution by atom  $j$  to the electron density to the electron density at atom  $i$  at a distance,  $r_{ij}$  (Oh and Johnson, 1988:471-472). For the potentials used in the present work, the chosen form of the repulsive potential is

$$\Phi_{km}(r_{ij}) = \Phi_{e,km}(r_{ij}/r_{e,km})^{-\gamma_{km}} \quad (5)$$

and the electron density,  $f$ , is

$$f_m(r_{ij}) = f_{e,m} \exp(-\beta_m r_{ij}/r_{e,mm}) \quad (6)$$

where  $\beta$  and  $\gamma$  are constants and  $r_{e,mm}, r_{e,km}$  are scaling factors to make the exponent dimensionless (Sabochnik and Lam, 1990:7-8).

The force on the atom is calculated as the negative value of the partial derivative of the total potential energy on the atom

$$\bar{F}_i = - \frac{dU(\bar{r}_i)}{d\bar{r}_i} \quad (7)$$

To avoid wasting computer time by calculating the forces between atoms which do not interact, atomistic simulations set up a 'neighbor list' for each atom. The neighbor list specifies which atoms will interact with each other. The list is periodically updated during a run to account for atoms moving. Another computer time saving method is to set the force on atom  $j$  from atom  $i$  equal to the negative force on atom  $i$  from atom  $j$ . This avoids calculating the same force twice. Once the force between the atoms are known, the equations of motion are solved. The equations of motion cannot be solved analytically for realistic interatomic potentials, and thus are solved numerically.

Because the forces on an atom depend on the number of neighbors it has, atoms on a vacuum only see half the forces that an atom on the interior would experience. Since it would use an inordinate amount of computer time to run a system of a million atoms, boundary effects are minimized by the use of periodic boundaries, in which the system is surrounded by copies of itself. Thus, atoms on the edge 'see' an atom across a boundary and react accordingly. If the atom crosses a boundary during the simulation, its 'image' will enter the simulation volume across the boundary opposite the one crossed by the initial atom.

Five state variables are present in each molecular dynamics simulation: volume, pressure, number of particles, temperature and total energy. For any MD simulation, three

of these variables are held constant. In this study, the volume, number of atoms and system temperature are fixed, and the other two properties are calculated. The potential energy is calculated using equation (1). The kinetic energy (K.E.) and temperature are related by

$$K.E. = \frac{3}{2} k * N * T \quad (8)$$

where  $k$  is Boltzmann's constant,  $N$  is the number of atoms in the system and  $T$  is the absolute temperature. The temperature is held constant using the extended system method (Nosé, 1984).

After the forces and temperature are determined, the pressure of the system is calculated

$$P = \frac{NkT}{V} - \frac{1}{3V} \sum_{i < j} \frac{du(r_{ij})}{dr_{ij}} \quad (9)$$

in this equation,  $V$  is the volume of the system, the derivative of the potential energy is the magnitude of the force of atom  $j$  on atom  $i$  and  $r_{ij}$  is the distance between atoms  $i$  and  $j$ . If the pressure is held constant rather than the volume, the system will expand or contract with an increase or decrease, respectively, in pressure.

Molecular statics calculates the forces between atoms in the same manner as MD, but instead of solving the equations of motion, MS uses energy minimization routines. At the end of a molecular statics run the atomic positions should be such that the potential energy of the system is

minimized. Simply put, as an atom passes through its position of minimum potential, its acceleration and velocity of opposite sign. When the product of the velocity and acceleration becomes negative, the velocity is set to zero. The atom begins to regress along its path until the product of the acceleration and velocity becomes negative again, and so on. Since discrete time steps are used, the chance of the atom coming to rest precisely at its lowest potential configuration is low. Hence, a molecular statics run is stopped when the maximum force on any atom is below a given tolerance.

Monte carlo methods are usually used for a system of atoms in a fixed volume at a constant temperature. The Metropolis monte carlo technique goes as follows. The total energy of the system is calculated using the interatomic potentials. An atom is chosen at random and moved to a new position. If the energy of the system decreases the move is accepted. If the energy increases by less than an amount proportional to  $\exp(-E/kT)$ , where  $E$  is the energy,  $k$  is Boltzmann's constant and  $T$  is temperature, the move is accepted. Otherwise the move is rejected and the system returned to its previous configuration. If a statistically significant number of moves are used, average values of state variables calculated by MC are equivalent to those

found by molecular dynamics. However, since the equations of motion are not solved, monte carlo techniques are used only to find static properties. (Haile, 1980:6-7)

DYNAMO. DYNAMO is the atomistic simulation computer code used for this study. DYNAMO uses molecular statics to perform energy minimization calculations (molecular statics), and molecular dynamics or monte carlo (MC) methods to study atomic motion. The user specifies parameters, such as desired temperature, length of run and operating method (MS, MC or MD), in an input file read by DYNAMO. DYNAMO uses a fifth-order predictor-corrector routine to solve the equations of motion in molecular dynamics numerically. Since the MD routine steps forward a finite time in each step, the behavior of the system and its properties (energy, volume, etc.) with respect to time can be studied. During each step of a monte carlo run, a random atom is selected and moved a certain distance which depends on the input temperature of the system. After the atom is moved, the total energy of the system is calculated. If the energy of the system decreases, or increases within specified tolerances, the move is allowed; otherwise the position of the atom remains unchanged. Monte carlo is used to calculate the properties of canonical ensembles.

The user may also determine if a new lattice is created for the run by specifying the unit cell, atom positions within the cell, type of atom at each position in the cell

and number of unit cells in each direction. If continued study of previous work is desired, a restart file from a previous run may be read by the code and used as the initial atomic configuration, instead of creating a lattice for a new run. Restart files are included in the standard output from a DYNAMO run and contain information about the system at the end of the run in which the file is created. The total number of atoms, atom types, physical size of the system and the positions and velocity of each atom are contained in the restart file.

Another output from DYNAMO which is extremely important to this work, is the trajectory file. It contains the same data stored in the restart file, but the trajectory file saves this information at several times during the simulation. By plotting the trajectories of an atom over several thousand time steps, one may make qualitative judgements about the phase of the material. That is, a liquid will move randomly and over relatively great distances whereas a solid will remain within a short distance of its original position.

The third output from DYNAMO is the printout file. This file stores the properties of the system at specified intervals. The properties include the time, total system energy during the time step, and the instantaneous and average values of kinetic energy, potential energy, temperature, volume and pressure.

### Crystal Studied

The crystal used in this simulation is an intermetallic compound, CuTi. The CuTi is a body-centered-tetragonal crystal, which can be visualized as a cube with one atom centered inside a box and eight other atoms placed so their centers lie on the corners of the box. For this simulation, individual layers of atoms lie in the x-y plane and are stacked in the z-direction, two copper planes lying on 2 titanium planes (see Figure 1). The choice of crystal

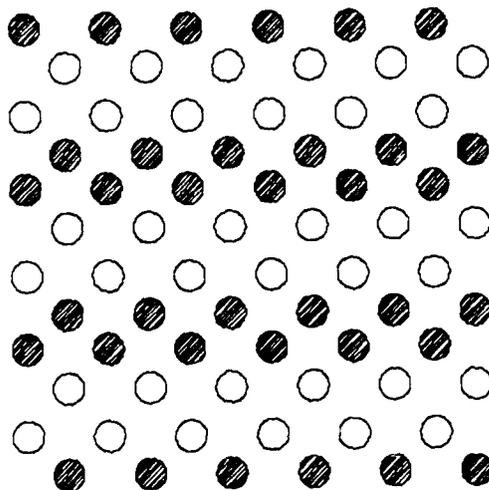


Figure 1, CuTi Crystal

size is not arbitrary; the system needs to be large enough to study the interface, yet small enough to minimize required computer time. A long, thin crystal is chosen to reduce boundary effects along the x-axis while observing the interface. Y- and z-axis boundary effects are reduced, but not necessarily eliminated, by making the crystal periodic in the y and z directions. A system consisting of 1080

atoms (30 atomic layers, each 6 by 6 atoms) is studied since the code would not need to be modified to accommodate this size crystal and it is long enough to allow study of the interface over meaningful times (>20000 steps). If the interface crosses the crystal too quickly little or no useful data is obtainable.

The Cu-Ti system is created using the lattice creation capability of DYNAMO. The unit cell consists of four titanium atoms at the bottom "corners" of the cube, a copper atom centered among the four Ti atoms in the x-y plane and one atomic layer above them in the z-direction the titanium. Two similar layers with the atom types reversed are placed above the copper atom to complete the unit cell. The system used is formed by forming a block of 30x6x3 unit cells of CuTi.

### Analysis Methods

Both qualitative and quantitative techniques were used to analyze the output from the simulation runs. Qualitative methods, including trajectory plots and atom position plots, were used to make a rough estimation of the interface location and the chemical order or disorder of the recrystallized CuTi. Mean square displacement, atomic density distributions and order parameters were used to quantify the position of the interface and the phase of the

material in the melt area. A comparison of the analysis methods (excluding the mean square displacement) is in Appendix A.

Trajectory Plots. Trajectory plots use the data in trajectory files to produce a picture of the path an atom follows during the run. The user can specify the time during which the atoms are followed, the viewing direction and a slice of the system to view.

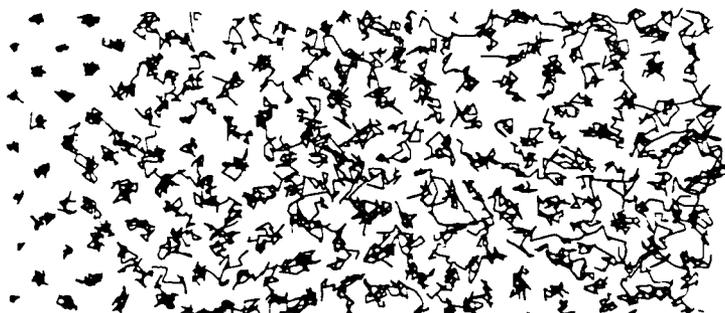


Figure 2, Sample Trajectory Plot

A sample trajectory plot is shown in Figure 2. The dots on the left hand side of Figure 2 are atoms held in place by the code. The larger spots to the right of the fixed atoms are atoms in a solid phase. Their small trajectories result from vibrational motion. At higher temperatures the spots will get larger, at lower temperatures the spots will

decrease in size. The area right of the solid is liquid, evidenced by the long pathlengths and lack of visible structure.

Trajectory plots are the easiest of the analysis methods to read, but they must be used with caution. If the time span used in the plot is too small or the time steps too large, atoms that are in liquid phase may appear to be an amorphous solid because there are not enough points to plot. The atom in the liquid will seem to move only a short distance. On the other hand, viewing the trajectories over too much time is equally undesirable. Similar care must be taken when selecting the slice thickness. Too thin a slice will result in a sparse plot revealing little information. If the slice is too thick, the overlapping trajectories of atoms along the viewing axis will smear the definition of the plot. Because of these limitations, trajectory plots are only used for a crude estimate of interface position.

Atom Position Plots. Atom position plots, also called atom projection plots, show a snapshot image of the system. These plots use the atom position information contained in the restart files to plot the atoms in their relative positions. The user may specify the viewing angle, the orientation of the system, and the depth and thickness of the slice viewed. A sample projection file is shown in Figure 3.

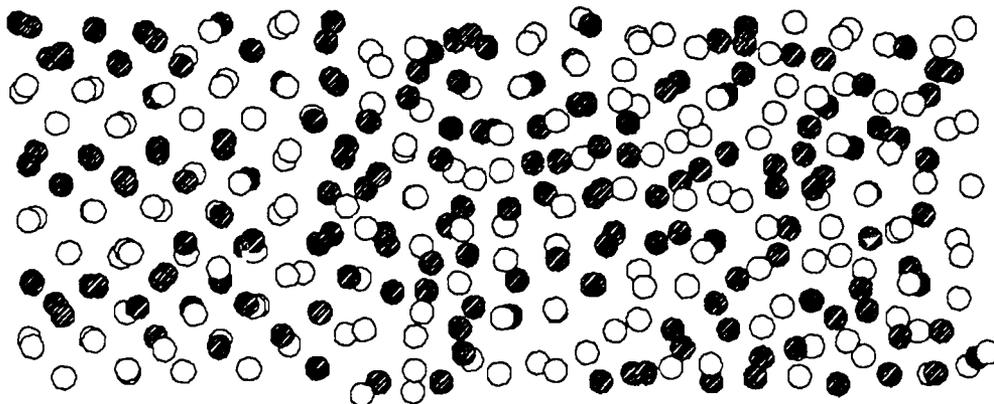


Figure 3, Sample Projection Plot

The filled circles in the projection plot represent titanium atoms, the open circles are copper. Moving from the left boundary to the right, three distinct regions are seen in the crystal. The three layers on the left border are held in place by the code as shown by the rigid structure. Order is evident in the next six atomic planes to the right, but much looser because the atoms have moved. Antisite defects, when two atoms of different kind change places, are also present, an example being the fifth atomic layer from the left. At the top of this layer, a copper-titanium pair are seen where a Ti-Ti pair are expected.

Projection plots are useful to see defects in the crystal, such as vacancies or antisite defects, and to see if the system shows structure. The plots are not useful to

determine the position or movement of a liquid-solid interface because it is not possible to determine if a disordered region is a liquid or an amorphous solid.

Mean Square Displacement (MSD). An atom's mean square displacement is the square of the vector distance the atom moves from its starting position over a specified time. To calculate the mean square displacement, the system is divided into groups of atoms, each one atomic layer or 1.5 angstroms ( $\text{\AA}$ ) thick, spanning the y-z plane. The user specifies the trajectory file to be used and the starting and ending times of interest. The squared displacements of all atoms in the group are summed and divided by the number of atoms in the group at the initial time. If an atom from group 12 crosses the boundary into group 13 during the MSD calculation, it is still considered to be part of group 12 during the remainder of the calculation.

The MSD is a method of determining the position of the interface and the phase of the system. The self-diffusion coefficient for liquids is several orders of magnitude higher than for solids, so atoms in liquids move farther than in solids. In this study, the mean square displacement is averaged over several groups in the apparent liquid region in a trajectory plot. The location of the interface is defined as the position where the MSD is one-half the average group mean square displacement of the liquid. To identify the phase of the region, average group MSDs are

calculated for the groups in the region as a function of time. The MSD will approach a constant value over time for solids, but will increase linearly with time for liquids (Haile, 1988, 36).

Atomic Density Distribution. Atomic density distributions show the distribution of atoms along the x-axis of the system. The system is broken into smaller groups than for a mean square displacement, each having a thickness of  $.375 \text{ \AA}$ . The number of atoms in each group is plotted against the midpoint of the group. If the system is crystalline, the distribution will have high, sharp peaks one or two groups wide, and deep valleys of very few to no atoms. An amorphous or liquid system will be more level than the crystal.

Order Parameter. The order parameter is a way of measuring the crystalline nature of a system. The order parameter is found by

$$\rho_{gk} = \frac{1}{\Delta t N(N-1)} \sum_{i \in g} \sum_{\substack{j \in g \\ j > i}} \cos\left(\frac{2\pi}{\lambda_k}(r_k^i - r_k^j)\right) \quad (12)$$

$\rho_{gk}$  is the order parameter of group  $g$  in the  $k$  direction,  $N$  is the number of atoms in group  $g$ ,  $\lambda_k$  is the distance between atomic layers in the  $k$  direction (the lattice constant), and  $r_k^i - r_k^j$  is the distance from atom  $i$  to  $j$  in the

k direction.  $\Delta t$  is the number of trajectory files used when calculating an average order parameter for a given time during a run.

As a system becomes crystalline, the average distance between atoms in a given direction will approach the lattice constant for that direction,  $\lambda_k$ . For a perfect crystal  $\rho_k = 1$  for all directions. If the crystal is heated, the order parameter will be slightly less than one, since the atoms will move. The interface between crystalline and amorphous regions is defined here as  $\langle \rho_{yz} \rangle = 0.2$ ,  $\langle \rho_{yz} \rangle$  is the average of the order parameters in the y- and z-directions.

## Procedure

### Overview

The type of approach used was required not only because of the limited research time, but also due to the limited amount of time available on the Ohio Supercomputing Center Cray Y-MP. The crystal was created and heated to the temperatures to be used in the freezing runs. The liquid-solid interface was created using a modified monte carlo subroutine and the system was cooled various temperatures. The output was analyzed and decisions to either continue at the current temperature or to lower the temperature were made.

### Liquid-Solid Interface Creation

After the crystal was created, it was heated to 1000 K, 1100 K and 1200 K to prepare it for the next phase: melting part of the crystal to set up the interface. The system was minimized after heating to restore the Cu-Ti to a perfect crystal lattice. The y- and z-boundaries were fixed at their post-minimization values so no shear stresses will occur between the held and free atoms when the atoms are released for freezing runs. The x-boundary was extended to  $90\text{\AA}$ , creating a  $40\text{\AA}$  void along the x-axis to allow the system to melt. If the x-boundary was fixed at its

minimized value, the system would not melt because the system could not expand, thus maintaining the atoms in their lattice. The crystal was now ready to create the interface.

The liquid-solid interface was made using the monte carlo routine in DYNAMO, modified as follows. Atoms with an x-coordinate less than  $9.0 \text{ \AA}$  were held in place. Melting was accomplished at 3000 K, much higher than the experimental melting temperature, to reduce the time required to set up the interface. The output from the melting run is hereafter referred to as "the melt".

#### Resolidification Using Molecular Dynamics

After the liquid-solid interface was set up, molecular dynamics was used to resolidify the system. The boundaries remain fixed at the same values as the melting runs. The first three atomic layers from the x-axis are held to simulate a solid CuTi crystal extending in the negative x-direction. If the atoms are not held, the system may melt completely because it sees a void for x less than zero due periodicity and the large void introduced in the melting procedure (total system melting was observed in the initial recrystallization attempts).

The first step in recrystallization was to reduce the temperature to the value corresponding to the boundary lengths used during melting. This was accomplished using only 2000-4000 steps to lessen recrystallization during the

cooling. In all the runs described here, a time step was defined as  $2 \times 10^{-15}$  seconds. After the crystal was cooled, several runs are completed over longer times, 10000 or 20000 steps. After each run was completed, the output was examined to determine the location of the interface, the order of the atoms in the solid, and the phase of the disordered volume (liquid or amorphous solid). If the interface has not moved noticeably, the temperature was lowered 100 K, and the system run again. The means of analysis are covered in the following chapter.

Recrystallization Attempts. Based on the work by Wood and the experimental value of the melting point of CuTi, 1200 K was the temperature used for the first solidification attempt. The crystal was held at 1200 K for 20000 time steps. The subsequent plot of the trajectories showed the crystal had completely melted. A similar set of runs made at 1100 K also produced a melted system, so a decision was made to hold three atomic layers during the crystallization runs. The rationale for immobilizing the layers was that the interface surface under study may be of such a high energy state that the system found it easier to melt than to maintain and build on the interface. Since monte carlo was not used for recrystallization, the forces on each atom and the atoms' velocities were set to 0 during the force calculations in molecular dynamics.

Starting from the melt at 3000 K, the 1200 K recrystallization attempt was repeated. The system was cooled to 1200 K in two separate runs: the first of 1000 steps to 2000 K and the second to 1200 K in 1500 steps. After cooling, the CuTi was held at 1200 K for 2 subsequent runs, one 10000 steps and one 5000 steps. Examination of the atom trajectories showed no noticeable movement of the liquid-solid interface. A plot of the atoms showed structure in the three rows held and in the two adjacent rows. The structure in the two free rows is seen because of the binding effect of the stationary rows. The structured region is limited to two rows due to the effective range of the interatomic potential. If the system would recrystallize at 1200 K it would take too long to see in terms of simulation, and hence computer, time. The time of the simulation at 1200 K was 35 picoseconds (ps).

The temperature was lowered to 1100 K in an attempt to recrystallize the system faster. In addition to the lower temperatures, the boundary lengths in the y- and z-directions were shortened to the edge lengths of an equilibrated 1100 K crystal. Again the runs were started from the melt at 3000 K and reduced to 1100 K in 2 runs of 2000 steps each. The initial cooling runs were longer to allow the shock introduced by squeezing the system to pass through the system. Three 10000 step computer runs were performed on the system at 1100 K. Analysis of the

trajectories and atom positions failed to show quantifiable movement of the interface, even though the system had been run for 68 ps.

The temperature was again lowered, to 1000 K, and the boundaries reduced accordingly. To reduce the computer time required in the initial cooling phase, the restart file from the first 10000 step run at 1100 K was chosen as a starting configuration for the 1000 K runs. No initial cool-down runs were performed on the CuTi; instead, the first run at the new temperature lasted 10000 steps. A quick overview of the trajectory plots revealed a small area near the  $z = 0$  plane appeared to crystallize early in the run, between 2000 and 6000 timesteps, only to disappear by the end of the run. The crystal appeared to form facets into the liquid instead of growing perpendicular to the interface surface (see Figure 4). This is similar to the faceting observed in silicon by Landman in the simulation of Si (111) (Landman, et al., 1988b). Although the crystal seemed to melt by the end of the run, its appearance was encouraging enough to continue at 1000K for 20000 more steps. The additional time at  $T = 1000$  K did not produce the desired results. More faceting was observed, but the facets would melt before they had grown large enough to sustain recrystallization. More runs at 1000 K were deemed unlikely to recrystallize the system.

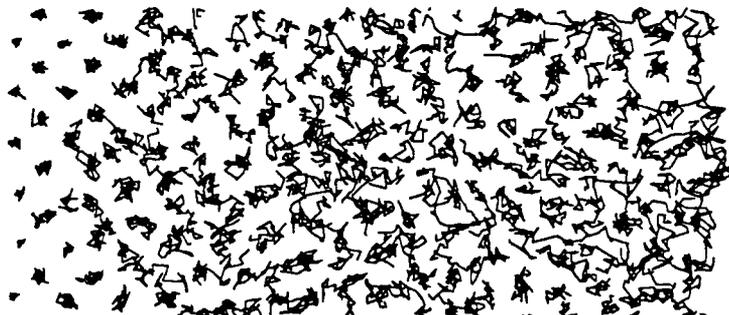


Figure 4, Trajectories,  $T = 1000$  K  
 $t = 32 - 36$  ps

The next temperature tried was 900 K, with corresponding boundary lengths. The CuTi was held at 900 K for 20000 timesteps using the output from the first 1000 K run as a starting file. At the end of this run (88 ps from the initial melt), two atomic layers of crystal appeared to have grown and remained at the end of the run. The system was held at 900 K for 129 ps more, which formed only two additional atomic layers of crystal. More crystal growth had been expected. The temperature was lowered 100 K once more in an attempt to freeze the system in an amorphous state.

The CuTi was held at 800 K for 40 ps. The starting point was the end of the first 1000 K run, 48 ps from the melt. After a the additional 40 ps, the projection plot of the final configuration showed no obvious movement of the

interface and trajectory plots indicated that the atoms in the melted region seemed to move less as the simulation progressed. A plot of MSD vs time for the disordered region (Figure 5) showed a linear increase in the MSD. It is not evident whether this is an amorphous solid, glass or liquid, since glasses do exhibit some liquid-like properties.

After failing to produce an amorphous solid at 800 K, the three layers of atoms that had been held were released. The output from the final 900 K run, 217 ps from the melt, was held for an additional 40 ps. Although 900 K was the intended temperature, the system was actually run at 818 K. Projection plots and trajectory plots still did not show the interface moving. Comparing the order parameters at 8 ps intervals through the run confirmed the interface had not noticeably moved.

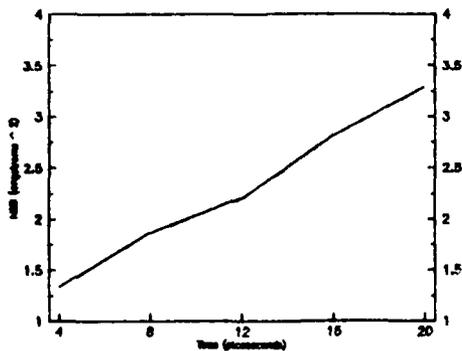


Figure 5, MSD vs Time, T = 800 K

A run at 773 K was set up and run for 80 ps timesteps in a final attempt to form an amorphous solid. However, analysis of the trajectory plots and projection plots showed a definite crystal growth in the system. The CuTi was run for an additional 80 ps at 773 K, and further crystal growth was noted. Figures 6a-c show the projection plots of the system at the beginning of the runs at 773 K, after 80 ps at 773 K and after 160 ps, respectively.

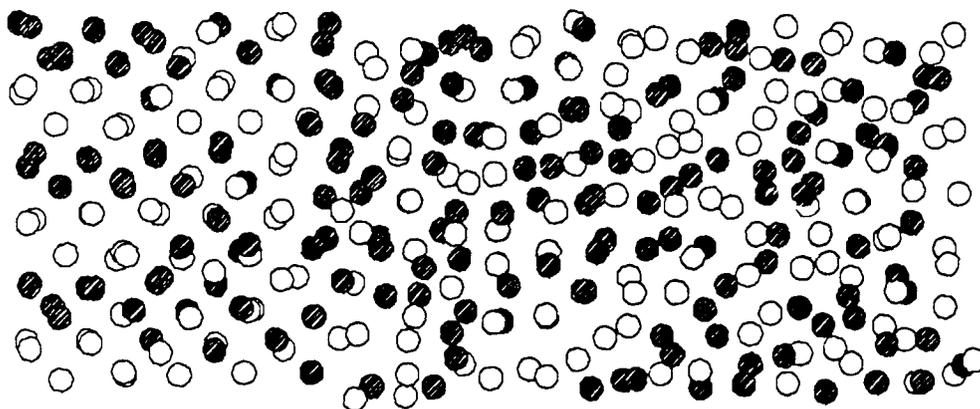


Figure 6a, Atom Positions at Beginning of 773 K Runs

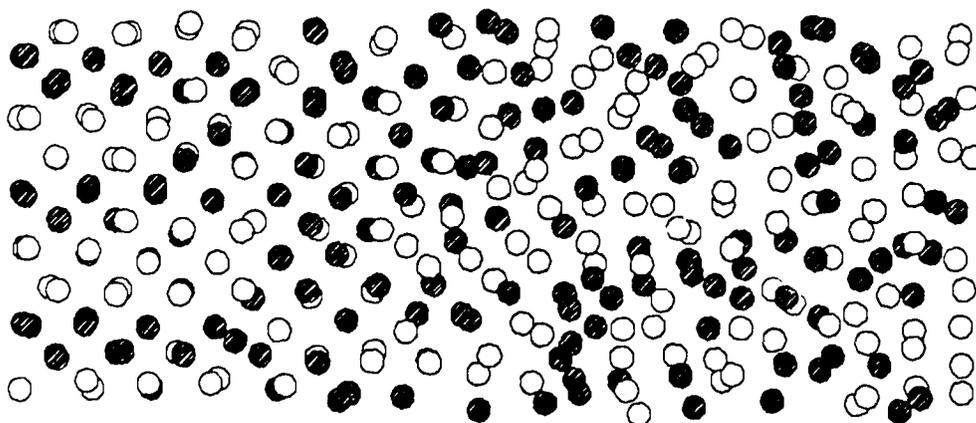


Figure 6b, Atom Positions after 80 Picoseconds at 773 K

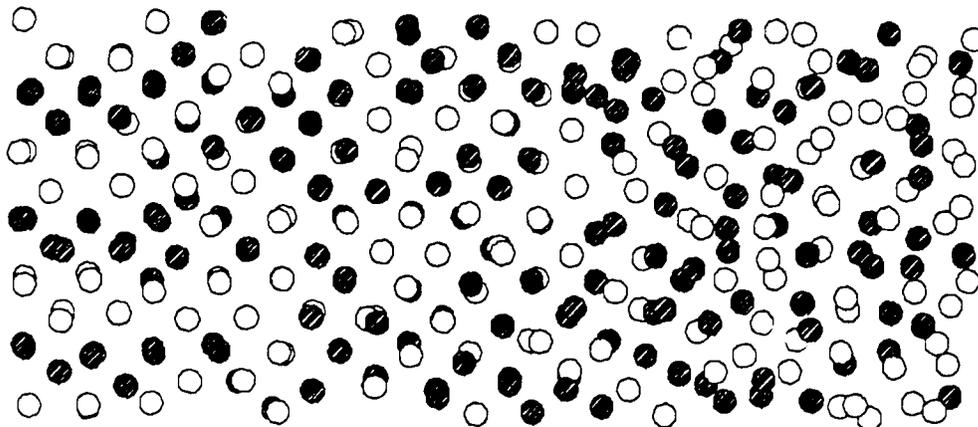


Figure 6c, Atom Positions after  
160 Picoseconds at 773 K

The crystal clearly grew from left to right, starting about one-quarter of the distance across the crystal and ending almost two-thirds across. The trajectory plots corresponding to each projection plot are shown in Figures 7a-c.

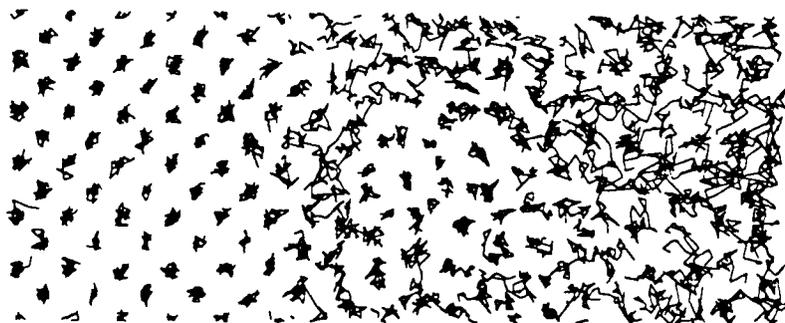


Figure 7a, Trajectory Plot  
0-16 Picoseconds,  $T = 773$  K

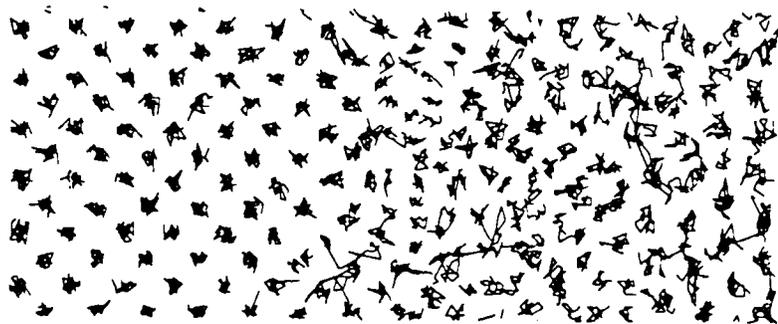


Figure 7b, Trajectory Plot  
80-86 Picoseconds,  $T = 773$  K

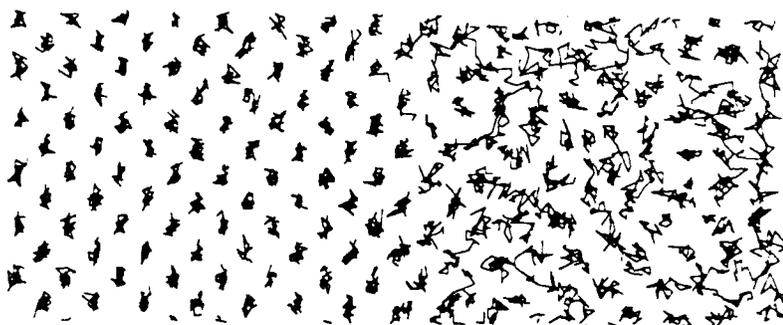


Figure 7c, Trajectory Plot  
144-160 Picoseconds,  $T = 773$  K

The trajectory plots also show the crystal grew from left to right, covering almost half the crystal in 160 picoseconds. The output from these runs was analyzed in greater detail to determine the interface velocity. This analysis is covered in Chapter IV.

## Analysis of 773 K Runs

### Estimate of Interface Velocity Limit

As seen in Figures 6 and 7, the CuTi appears to have recrystallized across a large portion of the system. To get more precise values for the extent of recrystallization and the velocity of the interface, more detailed analysis is required using atomic density plots and the order parameter. MSD calculations were unreliable for the 818 K and 773 K runs. Before this analysis was done, an approximation of the interface velocity was made using the MSD output from the initial 1000 K run and the 818 K run. An average mean square displacement was calculated over ten groups in the liquid region for five time spans. The diffusion coefficient was calculated for each  $\Delta t$  using Equation 11, and an average diffusion coefficient was found for the liquid region. The interface velocity was calculated using Equation 10 using  $\lambda = 1.5\text{\AA}$ . The results are shown in Tables 1 and 2. The velocity limit at 818 K is lower than the limit at 1000 K. This may be due to reasons covered in the chapter on previous work.

Table 1  
Interface Velocity Limit, 1000 K

$\Delta t$ (ps)	MSD ( $\text{\AA}^2$ )	D ( $\text{cm}^2/\text{s}$ )	Interface Velocity Limit (m/s)
4	$4.7 \pm 1.2$	$2.0 \pm 0.5 \times 10^{-5}$	
8	$8.9 \pm 1.2$	$1.9 \pm 0.4 \times 10^{-5}$	
12	$12.0 \pm 2.2$	$1.7 \pm 0.3 \times 10^{-5}$	
16	$13.3 \pm 2.2$	$1.4 \pm 0.3 \times 10^{-5}$	
20	$20.7 \pm 3.0$	$1.7 \pm 0.3 \times 10^{-5}$	
Average		$1.7 \pm 0.3 \times 10^{-5}$	

Table 2  
Interface Velocity Limit, 818 K

$\Delta t$ (ps)	MSD ( $\text{\AA}^2$ )	D ( $\text{cm}^2/\text{s}$ )	Interface Velocity Limit (m/s)
8	$3.9 \pm 1.1$	$8.2 \pm 2.3 \times 10^{-6}$	
16	$7.3 \pm 1.4$	$7.6 \pm 1.6 \times 10^{-6}$	
24	$11.5 \pm 1.9$	$8.0 \pm 1.3 \times 10^{-6}$	
32	$17.7 \pm 2.9$	$9.2 \pm 1.5 \times 10^{-6}$	
40	$18.8 \pm 4.1$	$7.8 \pm 1.7 \times 10^{-6}$	
Average		$8.2 \pm 1.7 \times 10^{-6}$	

Trajectory and Projection Plots, 773 K

Examining Figures 6 and 7, it appears the interface has moved approximately five atomic layers or 7.5 angstroms to the right during the runs. A closer examination of the projection plots shows that as the system recrystallizes it does not grow back to its initial configuration. Several anti-site defects are visible, but no point defects appear.

The anti-site defects occur because atoms entering incorrect lattice sites do not possess enough energy to break free, thus allowing a correct type of atom to enter. The trajectory plots in Figure 7 show small trajectories for the atoms in the disordered, as well as the ordered region. This could have two causes: 1) the time span of the trajectory plots was too short, or 2) the disordered region has glass-like properties. If 2) is correct, the high temperature would cause the system to be viscous like molten glass and still allow diffusive crystal growth. The trajectory and projection plots can only give a rough idea of the growth of the crystal; the other analysis techniques were used to calculate the interface position and velocity.

#### Atomic Density Plots

The number of atoms within a given group was plotted versus the center x-coordinate of the group at the beginning and end of the runs at 773 K. The plots are shown in Figures 8a-b.

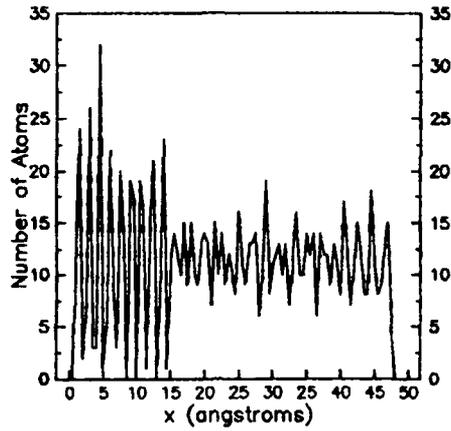


Figure 8a, Atomic Density  
 $t = 0$  ps,  $T = 773$  K

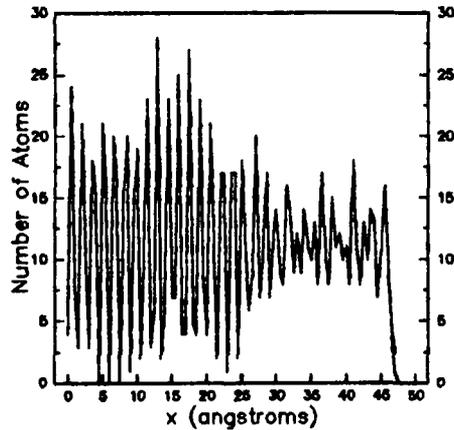


Figure 8b, Atomic Density  
 $t = 160$  ps,  $T = 773$  K

As the interface moves to the right, the number of sharp peaks and deep valleys increases. Each peak roughly corresponds to the position of a crystal layer. As the plot moves to more disordered regions, the difference between the

number of atoms in the peaks and valleys becomes less. The atomic density plots confirm that the system is growing in layers and not forming an amorphous solid. The location of the interface is found using the order parameter.

#### Interface Location Using Order Parameter

The order parameter,  $\rho$ , was averaged for every eight picosecond span for the two 773 K runs. That is, the average order parameters between 0 and 8 ps, 8 and 16 ps, 16 and 24 ps and so on, were calculated. The order parameter was calculated using Equation 13 for thirty five groups with widths of 1.5 angstroms. For analysis purposes, it is assumed the average order parameter occurred at the midpoint of each time span and each group. The y and z order parameters were averaged for groups bordering the interface. The location of the interface was calculated using linear interpolation to find  $\langle \rho_{yz} \rangle = 0.2$ . The interface was tracked for the duration of both runs and plotted vs time in Figure 9. Figure 9 shows the interface does not move with a constant velocity, similar to what Landman et al. observed for the recrystallization along the flat surface of silicon. The interface stays in the same vicinity for the first 52 ps grows at a very fast rate in the next 32 ps, remains constant for a short period and the grows again. The periods where no growth occurs may occur after one or two

layers grow then the atoms within those layers rearrange themselves to a lower energy configuration. The position of the interface remains constant until the crystal has stopped this rearrangement.

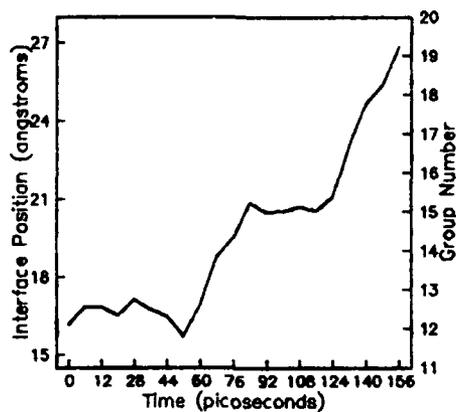


Figure 9, Interface Position vs Time  
T = 773 K

The positions at specific times during the run are used to calculate the velocity of the interface between two times. Time  $t = 0$  is the beginning of the first run at 773 K. The velocity is calculated simply by dividing the distance the interface moved (9.98 angstroms) by the time (152 ps). The average velocity of the interface over 152 picoseconds is 6.6 m/s, on the order expected in diffusion-limited growth. During the periods of rapid movement the interface reached speeds of up to 18 m/s (between 124 and 152 ps), but longer runs are needed to see

if these speeds are sustained for long times.

The simulated interface speed is .02 m/s above the velocity limit calculated earlier for 818 K. This actually agrees very well with theory, because the values for  $\lambda$  are not well defined. The system could be recrystallizing faster than expected since the atoms do not have enough energy to diffuse out of incorrect lattice sites and do not move before another layer freezes over them. The interface would not halt for long periods while the atoms in the crystal reorganized to a lower energy configuration.

What is interesting to note is the system refreezes in a chemically disordered state. If the low speeds are the result of diffusion-limited growth, the crystal should refreeze into its original configuration, since the recrystallization is slowed as atoms diffuse into the proper locations. If the type of atom entering the lattice site does not make any difference, as is apparently seen in the simulation, then the interface velocity should be on the order of collision-limited growth (~ 100 m/s). If an atomic layer requires a certain proportion of atom types be present in that layer but not in a specific configuration, a diffusive type growth would be observed. No analysis was done to determine if this is what occurred.

## Conclusions

The recrystallization and behavior of the liquid-solid interface of a CuTi body-centered-tetragonal crystal were studied using atomistic simulation. An interface was set up in the crystal using monte carlo and the system was cooled at various temperatures using molecular dynamics. Chemically disordered recrystallization occurred at 773 K: sustained recrystallization was not observed at higher temperatures and lower temperatures were not simulated.

Recrystallization appeared to occur as diffusion-limited growth at 773K based on the magnitude of the interface velocity taken from the simulation. If the growth was collision-limited, the speeds would be an order of magnitude higher. The recrystallization at this temperature is not truly diffusion-limited growth or the number of antisite defects would be significantly reduced, possibly to zero.

Although the growth appeared to be diffusion-limited, the regrown crystal was observed to be chemically disordered. The antisite defects arise due to the lack of mobility of the atoms in the amorphous region at the low temperature. Attempts to recrystallize the CuTi in its original configuration must be made at higher temperatures

to give the atoms in the liquid phase the energy required to move out of improper lattice sites before other layers form over them.

By no means was this an exhaustive study of the behavior and properties of the liquid-solid interface and recrystallization of CuTi, primarily because of time constraints. The lack of previous work on metal alloys was also hindering since no obvious starting point was available. Using molecular dynamics to simulate recrystallization of a concentrated metal alloy like CuTi was meaningful since no work has been published on it. The velocities resulting from the simulation at 773 K are within 20% of the limit at 818 K, which is good agreement considering the lattice constant is not well defined. Several questions arose during the study, such as: 1) If the recrystallization is governed by diffusion-limited growth, why are so many anti-site defects seen? 2) What is happening during the periods when the interface does not move? or 3) What is the thickness of the interface? A lack of both computer time and real time did not allow deeper investigation of these questions, but this study does provide a foundation for future work in the behavior of liquid-solid interfaces of CuTi.

## Appendix A: Comparison of Analysis Techniques

The four methods used to determine the location and movement of the liquid-solid interface during the 773 K runs are compared here to show they agree with each other. Figure A-1 is the plot of atom positions after 80 ps at 773 K. The atoms have some order in the first 11 to 12 atomic planes from the left boundary, beyond the 12 plane, no order is evident. If one atomic plane is approximately  $1.5 \text{ \AA}$  thick, the interface is between 16 and 18  $\text{\AA}$ . Figure A-2 is a trajectory plot of the system between 80 and 96 ps at 773 K. The solid region, denoted by the small spots, extends about 11 atomic layers, or about 17  $\text{\AA}$  into the system from the left. A plot of the atom densities vs distance from  $x = 0$  is seen in Figure A-3. The sharp peaks and valleys on the left indicate a crystalline region, the relatively smooth region is either amorphous solid, glass or liquid. The sharp, high peaks end approximately at  $x = 17 \text{ \AA}$ , which suggests that is the position of the interface. The final and most quantitative way of showing the movement of the interface is the order parameter. Table A-1 shows the y and z order parameters after 80 picoseconds at 773 K. The two order parameters are averaged and the interface is chosen where the average is 0.2. Although the average order parameter for group 4 is less than .2, this is because of movement into the vacuum to the left of the system not the

interface. The interface is in group 13, or between 17.5 and 19 Å. However, further investigation shows the center of mass has moved approximately 1.8 Å, so the interface is actually between 15.7 and 17.2 Å.

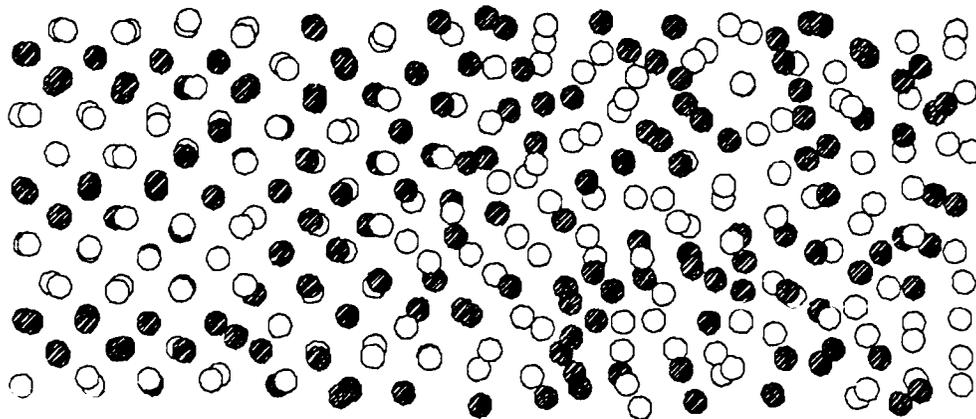


Figure A-1  
Atom Positions after 80 ps at 773 K

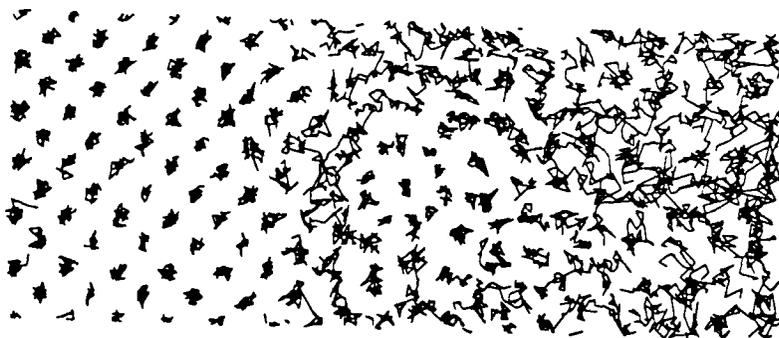
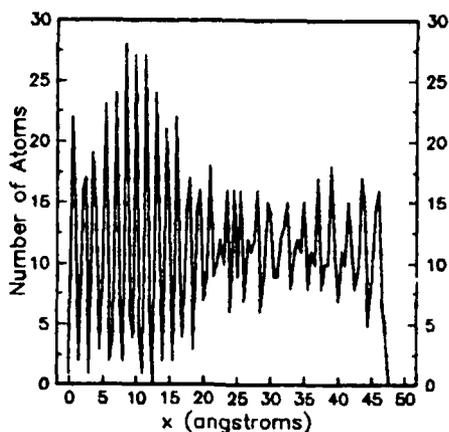


Figure A-2  
Atom Trajectories,  $t = 80-96$  ps  
 $T = 773$  K



Atomic Density at  $t = 80$  ps  
 $T = 773$  K

Table A-1  
 Order Parameters after 80 ps,  $T = 773$  K.

Group	Boundaries ( $\text{\AA}$ )	y	z
1	-0.5 1.0	0.26147	0.11005
2	1.0 2.5	0.46975	0.27542
3	2.5 4.0	0.48089	0.34289
4	4.0 5.5	0.55569	0.43370
5	5.5 7.0	0.45443	0.43219
6	7.0 8.5	0.44540	0.51101
7	8.5 10.0	0.51584	0.45268
8	10.0 11.5	0.51741	0.47067
9	11.5 13.0	0.46813	0.44353
10	13.0 14.5	0.45740	0.45532
11	14.5 16.0	0.38969	0.40226
12	16.0 17.5	0.33424	0.37536
13	17.5 19.0	0.20544	0.18161
14	19.0 20.5	0.10207	0.06441
15	20.5 22.0	0.00370	0.01529
16	22.0 23.5	-0.00381	-0.01328
17	23.5 25.0	-0.02029	-0.00656
Time		Center of Mass ( $\text{\AA}$ )	
At start of run		x	y
After 80 ps		25.73126	9.36897
		27.54551	9.25278
			z
			9.47101
			9.39467

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Vita

Captain Craig L. Loisel was born on 18 November 1963 in Springfield, Illinois. He was the valedictorian of the 1981 graduating class at Brussels Community High School in Brussels, Illinois, and then attended the University of Illinois at Urbana-Champaign. He graduated with honors and was commissioned in the USAF after being selected as a Distinguished Graduate from the AFROTC program at the university. His initial assignment was to the Life Support Systems Program Office at Wright-Patterson AFB, Ohio. He was the program manager for two eye protection programs, Laser Eye Protection and PLZT Thermal/Flashblindness Protection, and was responsible for fielding the PLZT windows used by the first operational B-1B wing at Dyess AFB, Texas. After four years as a program manager he was selected to attend the Air Force Institute of Technology, School of Engineering in August 1989. He married Catherine Miller in June, 1990 and they are expecting their first child in May, 1991.

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