ME 556 Project Report

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Abstract

Grain size in a metal directly affects its material properties. Grain growth is a process that can be controlled to influence the grain size within a metal to achieve specific properties. Polycrystalline materials undergo grain growth at elevated temperature lower than the melting temperature. In pure aluminum the velocity of the grain boundary migration is sensitive to temperature. Velocity of the boundary, under certain conditions, is also a function grain boundary curvature, κ. Atomistic modeling methods are employed to model a U-shaped half loop boundary geometry in an aluminum bicrystal simulation of molecular dynamics. This geometry will result in a constant migration velocity. Prior to grain growth simulation lattice constants for pure aluminum are determined through separate simulations for temperatures of interest. Data from the grain growth simulations is recorded after an equilibration period of 1000 ps. Snapshots of the system during the grain growth simulation used to calculate the velocity of the grain boundary. An overall trend of increasing velocity is shown as the result of increased temperature and the trend of decreasing velocity is recorded as curvature increases. It is shown how this data could be used to calculate the activation energy for grain boundary migration. The results are consistent with those of another simulation.

1 Introduction

Grain size is a property that is frequently controlled in materials processing to achieve desirable material properties. Conservative grain boundary motion can be driven by grain boundary structure, specifically curvature. The system changes in free energy with a reduction in grain boundary area, which results in grain boundary migration towards the center of curvature [6]. This migration can be simulated using atomistic methods to determine the effect of curvature on the velocity of the grain boundary in a pure aluminum bicrystal undergoing grain growth. Temperature also plays a role in the velocity of boundary migration. The effects of temperature and curvature during grain growth can be simulated with atomistic methods, and the output of such simulations can be analyzed to determine the velocity migration and the activation energy. A single grain boundary will be simulated in pure aluminum to obtain snapshots throughout the process of grain growth. From these snapshot visualizations of the process of grain growth, the relationship between curvature and velocity and the relationship between temperature and velocity can be determined. Finally, the results will be compared to those of a previous simulation.

2 Background

2.1 Scientific Principle

Polycrystalline materials undergo the process of grain growth at elevated temperatures. In this process the smaller grains decrease in size and eventually disappear while the larger grains grow with an overall increase in average grain size as the process continues. Part of the process is the motion of grain boundaries. There are many factors that can contribute to grain boundary motion, the two which will be the focus of this paper are temperature and grain boundary curvature. The velocity of the grain boundary is senstive to temperature, that is $v \propto T$. Curvature, κ, also affects grain boundary velocity during grain growth under certain conditions. For a single grain, if all grain boundaries are isotropic and of the same interfacial energy, γ, then:

$$v = M_B P = M_B \gamma \kappa \tag{1}$$

Where M_B in equation 1 is the mobility that links velocity with the pressure, P, towards the concave interface [1]. κ is the radius of curvature of the concave grain boundary, and if the previous conditions are met then, $v \propto \kappa$.

2.2 Modeling Approaches

Grain growth will be modeled using atomistic simulation methods outlined in the following section. Figure 1 illustrates the grain boundary geometry that will be modeled. During grain growth this U-shaped half loop grain boundary causes a constant migration velocity.[2].

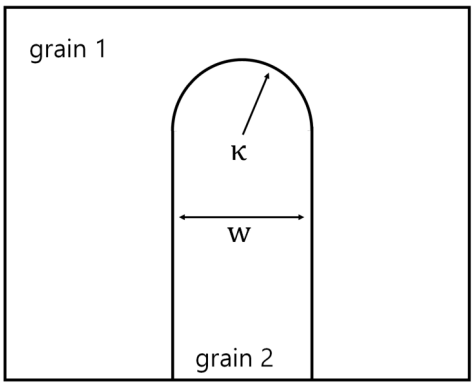


Figure 1: Schematic of bicrystal grain boundary. The width, w, is twice the radius of curvature, κ.

3 Methods

Prior to constructing the grain boundary simulations it was necessary to determine the lattice parameter for pure aluminum at the corresponding temperature for the grain boundary simulation. An equilibration was run in LAMMPS to determine the lattice parameter at those temperatures [4]. Table 1 shows the temperatures simulated and corresponding lattice parameters as determined by the equilibration. All simulations used an EAM potential [3]. The simulation cell and grain boundary geometry follows the schematic show in Figure 1. The width (x-direction) of the simulation cell was never less than $4w$ and the height (y-direction) of the simulation cell was never less than $5w$. The total length of the half-loop grain was no less than $3w$ [6]. The depth (z-direction) of cell was equal to the lattice parameter of pure aluminum at the simulation temperature. All simulations followed these criteria for cell dimensions.

Table 1: The grain boundary simulation lattice parameter used for each temperature. Determined by equilibration.

Temperature (K)	Lattice Parameter a (Å)
750	4.0982
800	4.1031
850	4.1076
900	4.1115

All simulations began with the generation of a symmetric tilt grain boundary in LAMMPS. Before any grain growth simulation, a minimization of the grain boundary structure was done in order to begin the grain growth simulation with a minimized structure [5]. Boundary conditions were periodic in x and z and shrink-wrapped in y for all simulations. The grain boundary motion simulations utilized the fix command to "freeze" the bottom three rows of atoms in the cell. This command set the component forces on these atoms to zero which did not allow them to move. This is shown in Figure 2 along with all other atoms thermostated, or set to desired temperature using the nvt command. From the starting point shown in Figure 2 simulations were run with timesteps of 0.001 ps until the loop had migrated from its starting position to the rows of fixed atoms.

4 Model Validation

When setting the temperature using the nvt command the Verlet algorithm requires that an initial temperature of double the desired temperature be set as the initial temperature. Over several time steps the energy of the system will fluctuate until it reaches equilibrium. The total energy per atom for each temperature was plotted versus the time step to determine once the system had reached equilibrium (Figure 3). Grain boundary motion begins as soon as

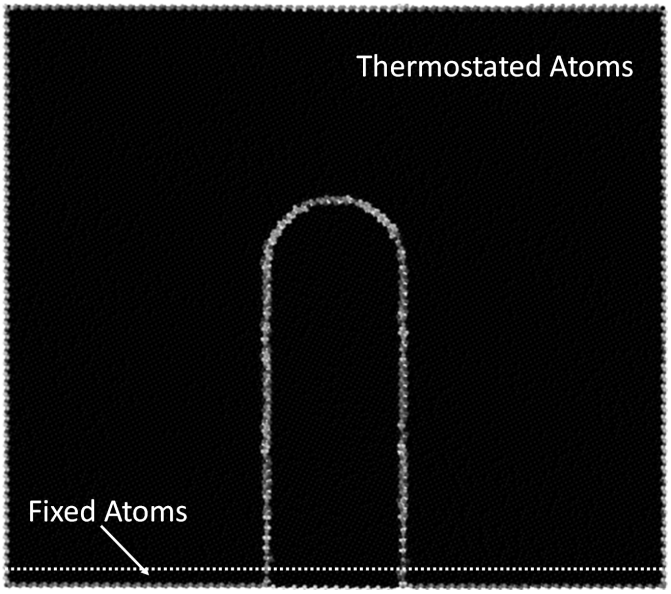


Figure 2: Snapshot showing the grain boundary simulation step at the initial timestep. The atoms below the dotted line are fixed and all other atoms are thermostated to the desired temperature.

the first time step, but to ensure results due to grain boundary motion only, with no influence from the equilibration period, only data from time step 1×10^6 and later was used in calculating the velocity of the boundary.

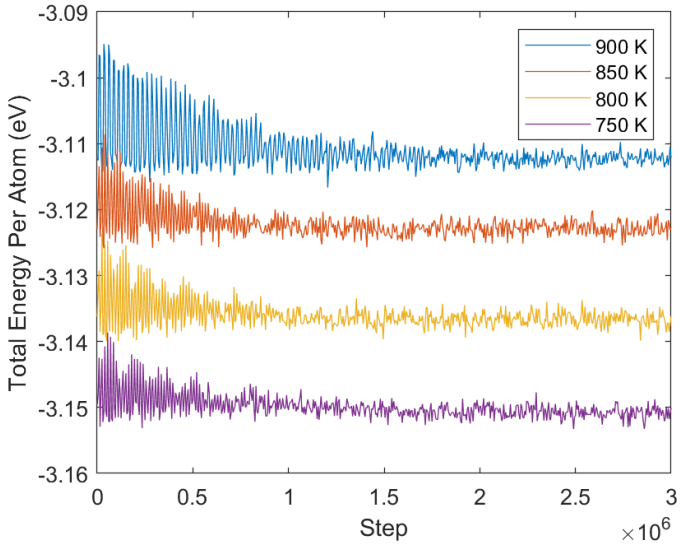


Figure 3: Total energy per atom versus step for various simulation temperature all with the same radius of curvature.

5 Results

Grain growth simulations were completed for four different temperatrues listed in table 1 all at $\kappa = 5a$. Four subsequent simulations were run at 750 K for $\kappa = 5a, 6a, 7a$, and $8a$. Temperatures were chosen that would allow for grain growth to occur but did not exceed 900 K due to the melting temperature of aluminum being around 930 K. Snapshots showing the evolution of the grain at different timesteps are included in Figure 4. Snapshots like those shown in Figure 4 were taken for all simulations and used to determine the velocity of the boundary. A Matlab script was used to determine the position of the curved end of the grain for several time steps. Velocity could then be calculate between time steps using the change in position divided by the change in time between snapshots. Velocity

for several time steps was calculated for each simulation and then averaged to obtain the overall velocity for grain boundary migration. Figure 5 shows the velocities for both the varying temperature and constant κ simulations as well as the constant temperature and varying κ simulations.

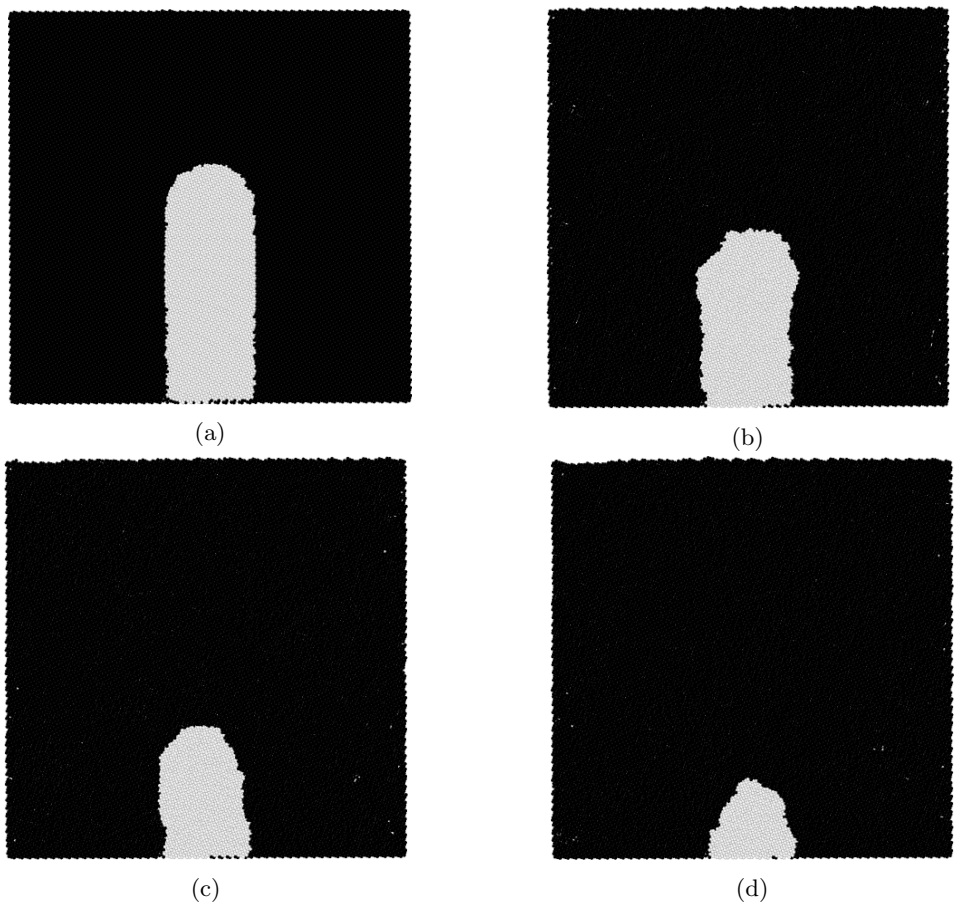


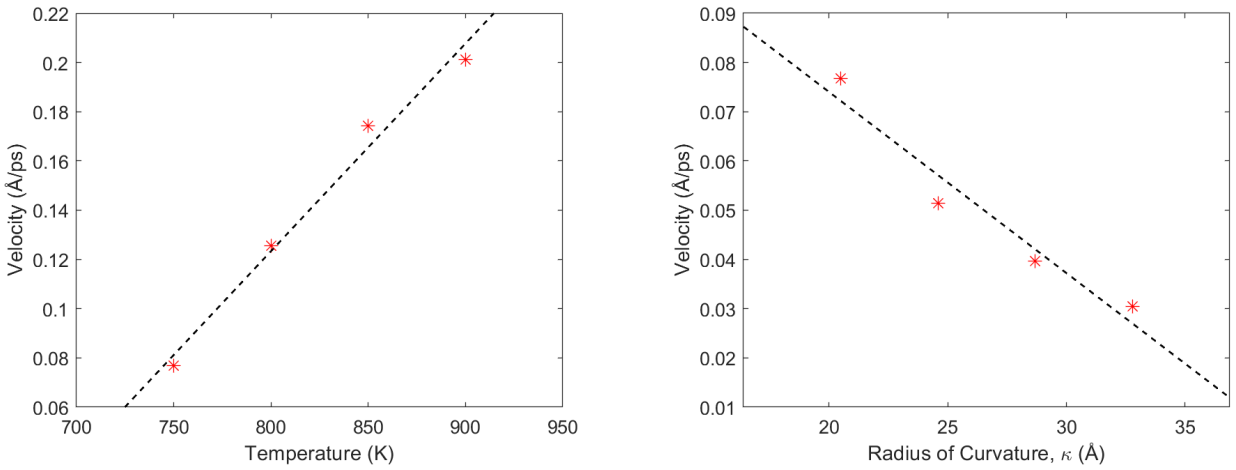
Figure 4: Evolution of grain growth simulation at 750 K at times a) 0 ps, b) 1000 ps, c) 2000 ps, and d) 3000 ps

6 Discussion

The velocity results shown in Figure 5 exhibit strong linear trends as the temperature/curvature increases. These results agree with those obtained by Upmanyu [6], which outlines three different migration velocity regimes: an initial transient regime that occurs at the beginning of the simulation, a steady state regime, and a final transient regime as the the boundary approaches the frozen rows of atoms towards the end of the simulation. The velocities measured likely occur in the steady state regime because of the linear trends, and the data used to calculate these velocities was taken after 1000 ps and well before the boundary could feel the effects of the frozen rows.

In the case of changing temperature, Figure 5a, the velocity of grain boundary motion increases as temperature increases. The increase in energy of the system results in faster grain boundary motion. This is consistent with the fact that grain growth is a temperature activated process that occurs at elevated temperatures less than the melting temperature of the metal. For the case of changing curvature, Figure 5b, the velocity decreases linearly as κ increases. This is also consistent with curvature driven grain boundary motion models [1]. Grains always grow towards the center of curvature. The larger the radius of curvature the slower the velocity of the boundary. A stable boundary will be a flat interface, infinite curvature, and will not migrate.

The data in Figure 5a can be used to extract the temperature dependence of grain boundary velocity. An Arrhenius plot of $ln(v)$ versus $1/T$ results in a linear relationship from which the activation energy for grain boundary migration can be extracted. The slope of the linear fit line is the activation energy; Figure 6 illustrates this principle. The activation energy will not be calculated here. This figure is used to show a useful application of the simulation results.



(a) (b)

Figure 5: a) Velocity plotted against temperature for four simulations of varying temperature and b) the velocity versus the radius of curvature for four simulations all at 750 K. The dotted lines show the trend as temperature/curvature increases.

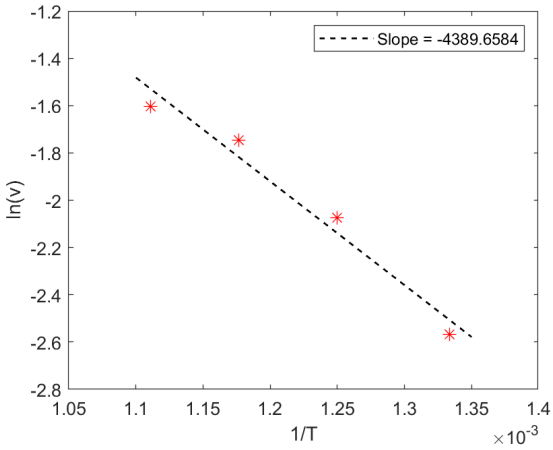


Figure 6: Arrhenius plot for the data present in Figure 5a. The slope values can be used to determine the activation energy of grain boundary motion.

7 Conclusions

1. The half-loop geometry grain results in uniform velocity of the boundary for grain growth simulations.
2. As temperature increases the velocity of grain boundary migration increases as well with a linear relationship, $v \propto T$.
3. As κ increases the velocity of grain boundary migration decreases with the relationship: $v \propto \kappa$.
4. The simulations are consistent with the results obtained by Upmanyu [6], particularly those in the steady state regime.
5. The results can be used to calculate the activation energy for grain boundary motion.

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