ME 556 Project Report

Ryan Melander
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Brigham Young University

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Abstract

0.1 Project Overview

Grain size is a process 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 [1]. This migration can be simulated using atomistic methods to determine the temperature dependence of grain boundary migration. A single grain boundary will be simulated in pure aluminum to obtain the necessary data (change to what the data is). The simulation will be carried out several times with varying curvatures to get the data. This data will be used to plot the activation energy of grain boundary migration.

0.2 Planned Methods

Detailed steps for simulation

- Setup u-shaped loop grain boundary in LAMMPS referenced in source [1].
- Length of the loop should be 3 times the width (w). Cell dimensions are at least $5w$ in the y-direction and $4w$ in the x-direction. The width, w, is 2κ, where κ is the radius of curvature for the curved portion of the loop.
- The loop will contain a lattice that has been rotated 30 degrees relative to the lattice outside the loop.
- Paper referenced uses the LJ potential. I will use the EAM potential for aluminum to model the behaviour better in the specific material. The LJ potential will be used for validation of the model and then swapped for the EAM potential.
- Boundary coniditions will be free for 3 sides of the simulation cell. The bottom edge, towards the center of curvature, will have 3 rows of atoms fixed to keep cell from rotating/translating.
- Run initial simulation on a single crystal to determine the lattice parameter to account for thermal expansion. (adapt lammps tutorial 3)
- Run molecular dynamics simulation on all the atoms that are not part of the fixed boundary maintaining a fixed temperature with the nvt command.
- Run molecular dynamics simulation for multiple curvatures at the same fixed temperature to determine curvature/mobility relationship

0.3 Preliminary Results

- Lattice parameter for Al at 300 K should be 4.06484 Angstroms (this is one tenth the length of the simulation cell from tutorial 3 which contains 10 unit cells).
- Ran grain boundary energy minimization to start the simulation with a minimized grain boundary. Then, the 3 rows of atoms on the bottom edge of cell were frozen by setting all forces to zero and the remaining atoms were thermostated at the simulation temperature using the nvt command.
- Figure 1 shows a simulation at various time steps throughout the grain growth process. Cell dimensions follow those listed in the planned methods section. Boundaries are periodic in the x and z-directions and shrink wrapped in the y-direction.
- The simulation was repeated at temperatures: 900 K, 850 K, 800 K, 750 K.

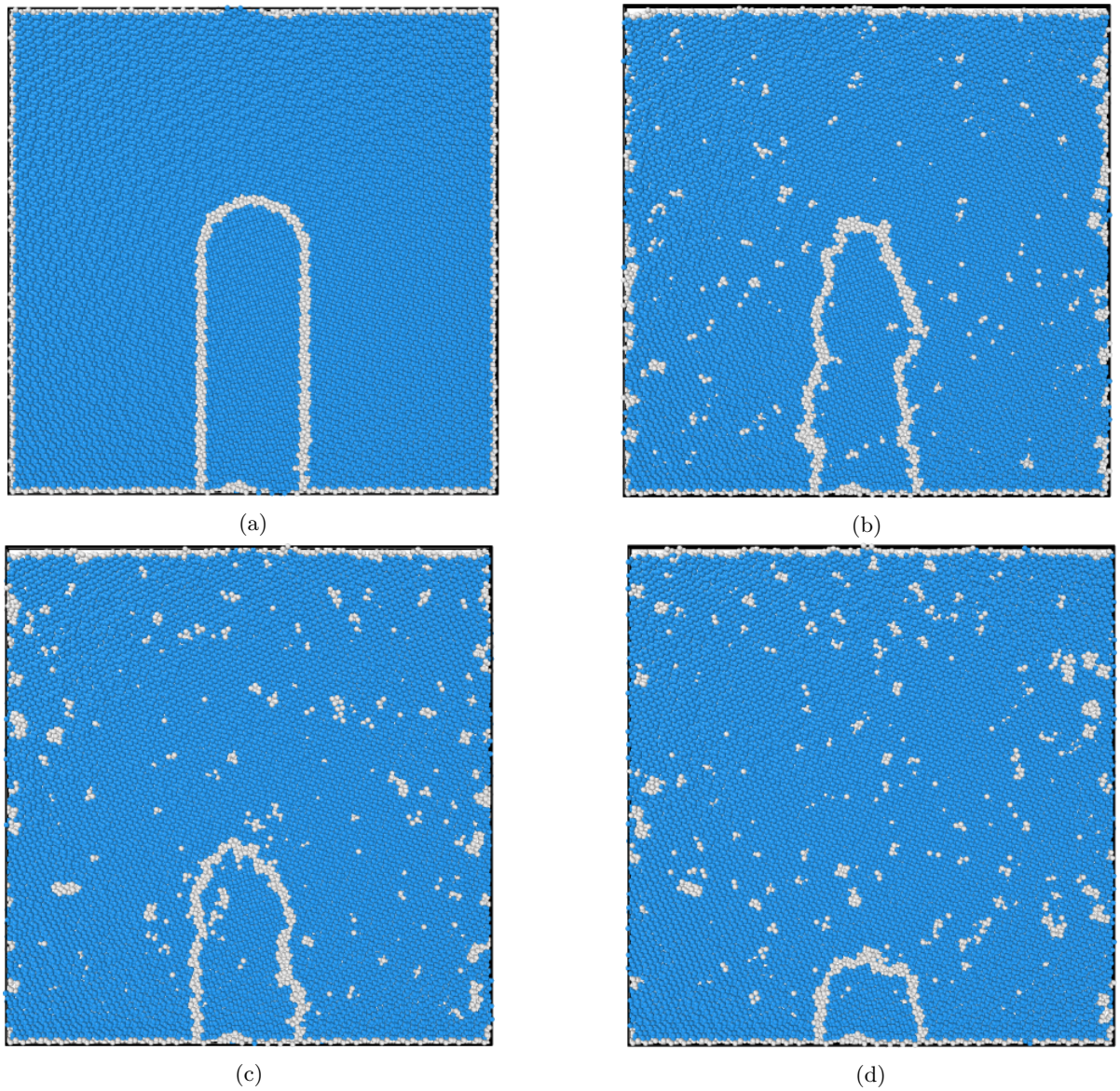

Figure 1: Grain growth simulation at 900 K. a) t = 0 b) t = 100 ps c) t = 250 ps d) t = 600 ps

Steps to complete project:

1. Rerun simulations with more output between time steps. Those already run were set to run for longer than is necessary for the grain boundary to migrate to the edge of the cell. For these temperature the grain boundary will have fully migrated to the edge between 600 and 1000 ps. This will also allow for more frequent dump files to better visualize the grain boundary motion.

2. Look into other thermo outputs (thermo_style). Currently I have the default outputs from the thermo command. Find a command related to energy or possibly another parameter that can be plotted and used to determine when the grain boundary is no longer migrating (stuck due to the edge of frozen atoms). Figure 2 shows a preliminary method that I thought could be helpful in determining the duration of time that the boundary is in motion.

3. Look into ovito modifications to get cleaner snapshots of the system (affine transformation) and to find a way to determine the number of atoms or area of a specific orientation (useful for determining the velocity of the grain boundary during migration).

4. The above two steps will be used to determine the velocity of the grain boundary in motion. The shape of the boundary is the typical shape used in simulations to produce a constant velocity. With the velocity of grain boundary motion for several different temperatures the activation energy for grain boundary motion determined. Produce a plot of $ln(v)$ vs $1/T$.

5. Varying the radius of curvature κ for a single temperature an plot: v vs κ

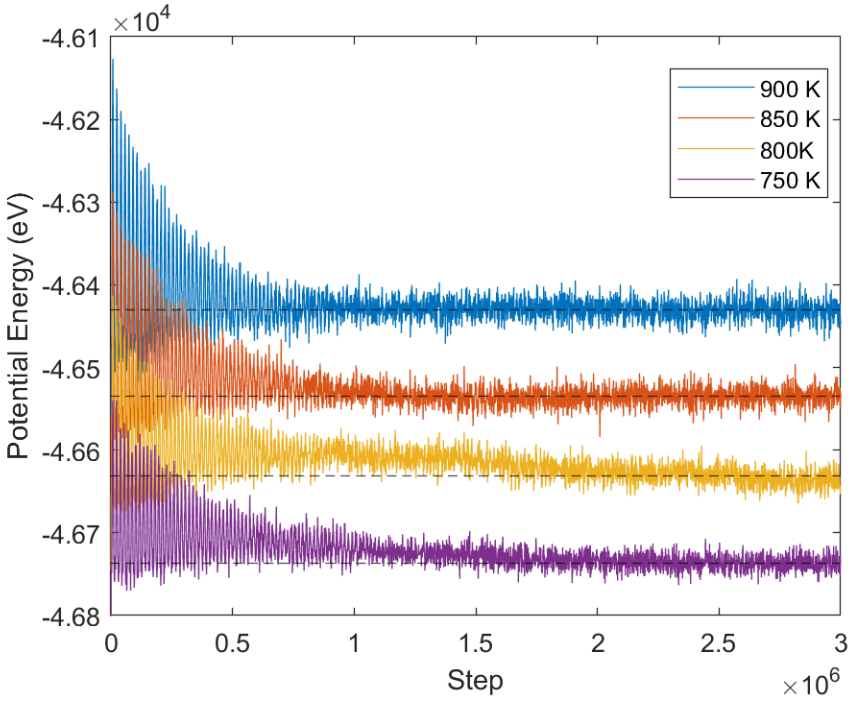

Figure 2: Potential approach to determining the duration of grain boundary motion. Once the total potential energy has reached a value close to the average equilibrium value (dotted lines) then the grain boundary motion is considered complete.

1 Introduction

2 Background

3 Methods

4 Model Validation

5 Results

6 Discussion

7 Conclusions

References

[1] M. Upmanyu, R.W. Smith, and D.J. Srolovitz. "Atomistic Simulation of Curvature Driven Grain Boundary Migration". en. In: *Interface Science* 6.1 (Feb. 1998), pp. 41–58. ISSN: 1573-2746. DOI: 10.1023/A:1008608418845. URL: https://doi.org/10.1023/A:1008608418845 (visited on 02/18/2022).