ME 556 Project Report

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Abstract

1 Introduction

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.

2 Background

2.1 Scientific Principle

2.2 Modeling Approaches

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).