Assignment 0 - Report 1: Energy and structure of a grain boundary in an FCC material using molecular dynamics

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April 27, 2022

1 Introduction

The calculation of energy and structure of a grain boundary (GB) in an face-centered cubic (FCC) material using molecular dynamics simulation as independent research is a pathway to present my capacity in independent research to solve research-like problems and evaluate my fit with the solid mechanics' computation field of study [1].

A crystalline structure of a material is a structure where atoms are spaced apart in a periodic array. As the atomic bond is metallic, there are some restriction on the number and position of elements that can be grouped in three principal crystal structures: face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal close-packed (HCP) [2]. This report focus on FCC materials.

The material can be classified as FCC when it has a cubic geometry with atoms located at each vertex and the centers of all the cube faces. A list of known FCC metals are copper, aluminum, silver, and gold [2].

Can observe a grain structure by looking at an FCC material under a microscope. The grain structure is an arrangement of grains or crystals. The grain is a three-dimension region occupied by a continuous crystal lattice. [3]. The outer edge of a grain region is defined as a grain boundary (GB). In the grain structure, this border separates each grain by a distance of one to three atoms. The measurement to characterize the energy of the GB is made with energy per unit area, representing the amount of work required to create the grain region [4]. This energy expressed by γ is influenced by the spatial position in reference to another grain and thermodynamic parameters as temperature, pressure, and chemical potential. To reduce the amount GB energy,could modify any of these parameters, and the crystalline structure would undergo a transformation process to find a new structure minimizing the energy of these boundaries [5].

2 Computation methods

Lammps was selected as a tool to develop the energy calculation and the structure of grain boundary. Lammps is designed as a computational engine for modeling interacting particles at any length scale [6]. With the correct parameters input and commands to compute, this tools provides numerical outputs that can be used to calculate the grain boundary energy. To visualise the result of crystal structures was necessary to use an application that covers molecular dynamics simulation. The visualization tool select was OVITO. OVITO is a 3D visualization software designed for post-processing atomistic data obtained from molecular dynamics [7].

The first part of Molecular Dynamic (MD) simulation calculates the lattice constant of Al and its cohesive energy in FCC lattice structure. The input script for LAMMPS was created based on

instruction provided by Mark Tschopp in his Github [8]. It initializing a individual FCC structure of the selected material and guessing an initial value to the lattice constant. After the script compute the energy of all atoms. The next step is to run a minimization to find the relaxation. The final step is to obtain The lattice constant as the size of structure after a relaxation process. The result found is a Cohesive energy (Ce) and Lattice constant (Lc) as follows:

$$Lc = 4.05\mathring{A} \quad , \quad Ce \ = -3.365eV \tag{1}$$

The next step of script is to create a random size region of the same FCC material and apply a stress and a energy minimization, to dislocate the grain boundary of grain regions. The Equation (2) calculates the grain boundary energy.

$$E_{gb} = \sum_{i \in V} \frac{E_i - E_0}{S_{gb}} \tag{2}$$

Where E_{gb}, the energy of grain boundary, is the summation of all atoms E_i in surface of grain (V), and E_0 is the bulk energy [9].

The script uses the same material and interatomic potential but now applied the first part of simulation in the two new regions. The regions are limited by a box of size 12.807225, 128.072245, 4.05 units of lattice. Each lattice was oriented in $< 031 >$ direction. After rotation the regions need to be displace and the atoms close to each other deleted. In this study two alternatives of distances to remove nearest atoms were run as case of study. The distances used was 0.35, and 1.5. The next step was apply the natural minimization process letting the system release the energy. As final part of simulation process, an expansion and contraction stress was applied in the grain boundary region to observe the dislocation and calculate the energy.

3 Results

As a result of this report the grain boundary energy was calculated in scenarios of different distance between atoms on the border of the grains. The Table 1 below shows the simulations, the parameter used is the minimum distance to remove atoms and the grain boundary resultant.

Simulation	**Distance Limit**	**GB Energy**
1	0.35	$564.166mJ/m^2$
2	1.5	$576.130mJ/m^2$

Table 1: Simulation results. Source: Author

The structure of grain changes as an effect of stress and relaxation process. The figure 1 shows the initial state of grain boundary and the figure 2 the structure after atoms remove by distance. After the relaxation applied, the structure changes the position of atoms reaching a better energy distribution. The new position of atoms are showed in Figure 3 and 4. Comparing these images is possible to visualize the differences in boundaries, because the distance limit of atom applied as initial state of simulation.

All scripts and results are committed in author repository in GitHub accessible in the link.

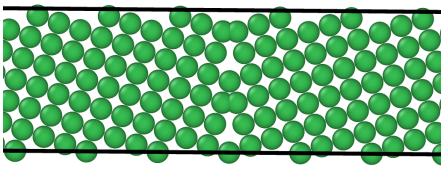

Figure 1: Initial position of lattice

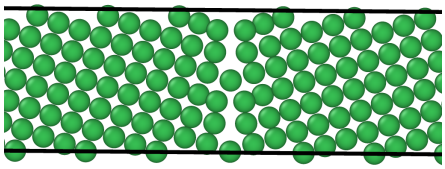

Figure 2: Lattice after overlap remove

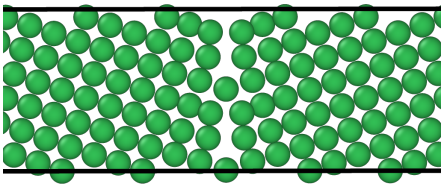

Figure 3: Grain boundary in simulation 1

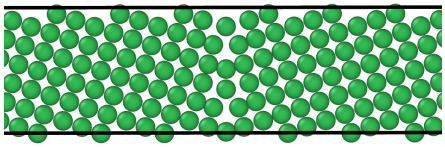

Figure 4: Grain boundary in simulation 2

4 Conclusion

In the material science field of study, the studies of material grains have already made a massive progress in describing atomic behavior and how it affects the mechanical components. After a brief review about grains, materials, and this behavior was possible to identify how complex it can be. This report covered the initial part of this study field by calculating the grain boundary energy between two grain of FCC material Al in a MD simulation with LAMMPS tools and presents the grain structure using the OVITO 3D visualization tool. The energy found on grains boundaries of Al FCC metal varies in order of the distance between atoms in grain boundary as can it modified in charge of any geometric and thermal parameters. It increases the computation class of this problem, whereas the degrees of freedom increases the computational complexity exponentially.

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