EVALUATION OF MECHANICAL PROPERTIES OF IRON USING MOLECULAR DYNAMICS SIMULATION

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Abstract

Simulation of Molecular Dynamics (MD) allows us to mimic the systematic variation of mechanical properties and energies beyond the capacity of experiment methods. By relaxing the stimulation cell along the X and Z-axis, the time taken to fracture was longer than usual in the symmetrical tilt grain boundary as the tilt axis was <110> at Σ value 3. The stress-strain graph values were obtained by using MD software Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) data. These values were plot with the help of PYTHON graphically. On application of strain along the y axis, stress also increased along the same axis with the increment in other two axes too i.e. X and Z-axis. The fracture of the tilt grain boundary was observed at the centre along its axis. At the 144^{th} step the fracture occurred while running the simulation. The simulation is run for 150 loops to provide the atomic relaxation in periodic cell boundary. With the help of LAMMPS, Per Atom Metrics is conducted in which properties of each atom is distinctively observed. The data from this simulation is colour mapped for better understanding of variation in properties. The potential energy is seen to be maximum in the close vicinity of the centre axis of simulation cell.

Keywords- Molecular Dynamics (MD), Coincident Site Lattice (CSL), Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), Open Visualization Tool (OVITO).

Introduction

The ever-increasing universal demand for energy efficient, secured, transportation, compatible systems for biomedical and safer applications requires developing modern materials with co-operative arrangements. The dominant properties of polycrystalline materials are majorly influenced by atomic details in relation with the crystallography of the grains and also with the grain boundary structure. The concept of “grain boundary

engineering" has led to an increment in the number density of grain boundaries with advantageous properties, while decreasing the number density of boundaries which have detrimental properties. Due to fracture of polycrystalline materials and mechanical behaviour is influenced mostly by their fundamental structure and grain boundaries, a basic understanding of relationship between the properties related to grain boundary and its structure is important to develop interface driven materials. Molecular dynamics (MD) studies have contributed to the evaluation of the atomic conduct of interfaces like solid–liquid interfaces, surfaces and grain boundaries as it is not easy to observe and to track the motion of atoms directly by experiment.

For example, Keblinski [1,2] explored the energy and amorphous structure of the grain boundary of Si by MD calculation and conferred the thermodynamic criteria for the stability. Wolf [3], Nakashima and Takeuchi [4] investigated the relation between the energy and also for the structure of the symmetric tilt boundary bcc-Fe.

In this paper, the fracture of tilt grain boundary is observed for BCC structure of iron during the simulation conducted using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) and OVITO (Open Visualization Tool) software. The stress-strain graph is also plotted using the output generated by running the input file for fracture of tilt grain boundary in LAMMPS. Also, per atom metric is performed which gives us the per atom properties. These will give us the angstrom number(a_0) value and the potential energy across the simulation done.

Experimental Methods

To perform the stimulation on LAMMPS(Large scale atomic/molecular massively parallel stimulation) we require a fundamental grain boundary data file 'Fe_110_sig3.txt' which consists data of the tilt grain boundary of Fe atoms and their respective locations as this will help to identify grain boundary locations in the Body centric cubic structure. The stress is applied along the x-axis and y-axis to perform the fracture under the 150 loops times step. After the fracture is done, we obtain a stress-strain data from the LAMMPS itself which is being analyzed and visualized to see the nature of the grain boundary in the Molecular Dynamics Stimulations. Again, the data file 'Fe_110_sig3' taken as fundamental for metric analysis on LAMMPS which help us to know the per-atom properties in stimulation cell, the data we get from it also visualized in pictorial cum rating graph with python codes.

3.1 Symmetrical Tilt Grain Boundary

In macroscopic world the polycrystalline materials are highly influenced by the nearby variations and properties caused by the impurities and defects. The effect of these impurities can either brittle or strengthen the grain boundary. In simple words we can perceive that a grain boundary is the interfaces between two grains or crystallites in a polycrystalline material, whereas it's procession part is called symmetrical tilt grain boundary (STGB). In cognizable we can say that symmetrical tilt boundary is generated by rotating two single crystals with respect to the tilt axis and connecting two crystals with the grain boundary plane also the tilt angle and the grain boundary plane must be parallel to each other during the moment of rotation. Hence the tilt angle **θ** is defined as the twice the angle of the φ. The Miller index (hkl) of the grain boundary plane is linked to the rotation angle with respect to the (*abc*) tilt axis as [5]:

$$cos\varphi = \frac{|\,bh - ak\,|}{\sqrt{(a^2+b^2)}\sqrt{h^2+k^2+l^2}}$$

Hence the tilt angle is,

$$\theta = 2\varphi = 2cos^{-1}\frac{|\,bh - ak\,|}{\sqrt{(a^2+b^2)}\sqrt{h^2+k^2+l^2}}$$

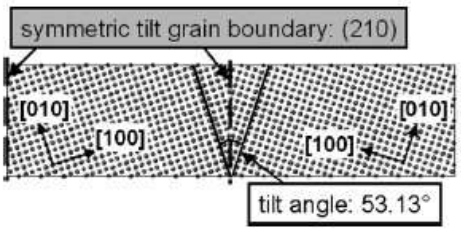

Figure 1: A schematic diagram of symmetric tilt grain boundary under condition of <100> tilt axis, an angle tilt of 53.15 degree

The above figure shows the structure of symmetrical tilt grain boundary in bcc phase defined by rotating two crystals 26.5 degree with respect to the <100> tilt axis and connecting them with plane (210) with tilt angle of 53.13 degree.

Similarly, we have selected the file of Fe with tilt axis of the <110> and with We know that at nanoscale atoms contains their own energy similarly there is a grain boundary energy. Because mechanical behaviour and structure of polycrystalline materials are often driven by the grain boundaries, the fundamental of understanding the relationship between grain boundaries and their associated relationship is important to create a interface dominant material.

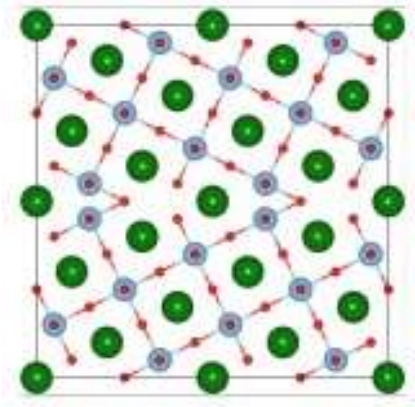

Figure 2: Symmetrical tilt grain boundary

The term grain boundary character is often used to describe five degree of freedom which are necessary to define grain boundary. The three degree of freedom are used to define the misorientation between two grains and where as other two are associated with the grain boundary planes. There are many studies which focus to develop to the characterize grain boundaries and their influence on physical properties of polycrystalline materials. These models utilise dislocation arrays, disinclination and coincident site lattice (CSL) describe local structure of grain boundaries. in CSL grain boundary grain of some atomic sites exactly coincident with some other atomic sites of other grain and these special sites are called coincident sites. It is believed that CSL grain boundaries low grain boundary energy because of good atomic fit. n spite of some softwares construct grain boundary to the best of our knowledge there is no universal and easy to use to generate grain boundary structure in high throughput fashion. So with the help of the LAMMPS we have generated the Grain boundary file which will be recognized as our data file here is a brief outline to build grain boundary that LAMMPS create for us: -

i. Calculation of rotation angle for a given Sigma value and rotation axis.
ii. Generate rotation matrix from the rotation angle and rotation axis.
iii. Calculate CSL matrix using rotation matrix and Sigma value.
iv. Generate two grains from CSL Matrix and combine them based on a given grain boundary plane to build a grain boundary.

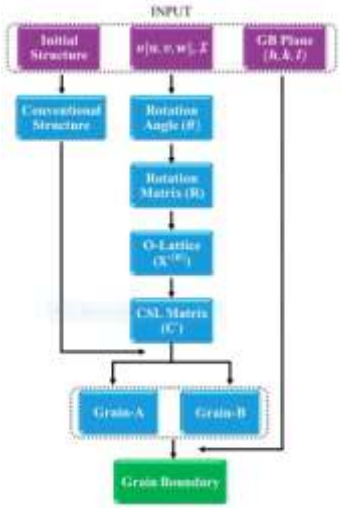

Figure 3: Complete building procedure of the periodic grain boundary

By completing the all the above procedures the grain boundary is obtain by LAMMPS. Whenever we mention a grain boundary it is represented by tilt axis and the sigma value many of us gets confused that what is the Sigma value [6] how it can be defined

$$\Sigma = \frac{Coincident\ Unit\ Cell\ Volume}{Rotated\ Unit\ Cell\ Volume}$$

In earlier studies it has been shown that grain boundaries with Σ3 are anti-thermal which means that temperature increases the grain boundary decreases and vice versa. The presence of Σ3 grain boundary effect on face centred crystalline mater it plays an important role in mobility of these boundaries to evolve nanoscale study. Surprisingly Σ3 grain boundaries with tilt axis of 110 are more thermally activated and showed high variation of mobility across their atoms range of boundaries. As considering we know that lower the distortion energy higher the value of Σ, which tend to have larger grain boundary area. The size of constraints of grain boundary limit the number of grain boundary planes orientations for these higher Σ CSLs. We directed our focus on low Σ grain boundaries, where many grain boundaries planes orientations provider better understanding how grain boundary energies varies entire stimulation. It is certainly noted that varies smoothly in Σ3 CSLs. In contrast to grain boundary energy, simple structure property relationships over the grain boundary plane fundamental zones for other grain boundary properties are not immediately obvious [7].

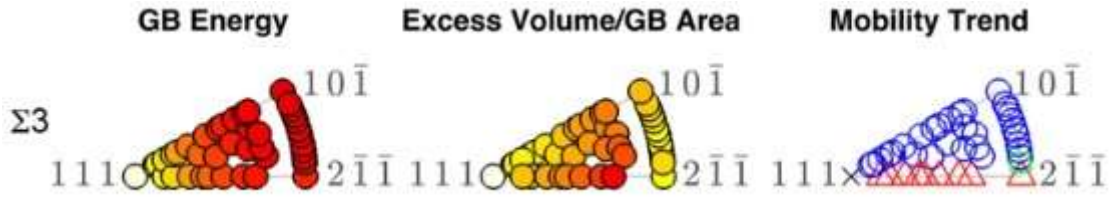

Figure 4: Correlation between properties GB energy, excess volume/GB area and Mobility trend.

In the above figure plots grain boundary energy excess volume per unit of grain boundary area and temperature dependent mobility trend in fundamental zone of each CSL. The excess volume per unit area for each CSL[8] generally correlates well with grain boundary energy trends. However even though this correlation exists notable exceptions the Σ3 grain boundaries show an initial increase in excess volume per unit grain boundary area drops back down at the curved fundamental zone boundary. In contrast excess free volume, the mobility trends do not appear to correlate with any other property. However, the mobility trends do not appear to be highly dependent upon the grain boundary plane orientation. It is particularly true of the Σ3 grain boundaries high percentage exhibited the thermally damned motion mechanism non-thermally where mobility inversely to the temperature. When the mobility trends of the Σ3 were finally plotted in the grain boundary plane orientation fundamental zone all of the thermally activated grain boundaries have normals that fall between the disorientation axis.

3.2 <110> Tilt axis

{111} boundary plane orientation is rotated about the <110> direction that lies in boundary plane, it creates series of grain boundaries that share common tilt axis <110> until 90-degree rotation reaches {112} orientation which is one of the symmetric incoherent twin boundaries. Many researches have shown that {111},{112}and {110} boundaries represent local energy minima in the Σ3 boundary plane space and that the structure and energy of general Σ3 are well represented by a model in which the boundaries facet along those low index planes. The <110> tilt boundaries facet on {111} and {112} planes [9].

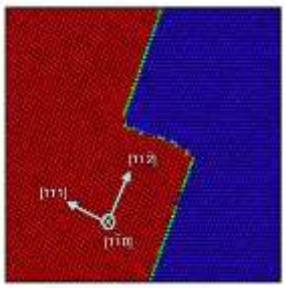

Figure 5: <110> facet along {111} and {112}

Taking each and every study in consideration it is noted that the <110> tilt boundaries found mobility with high inclination angle to the coherent twin, initially increasing the mobile facet normal gets closer to the direction of boundary motion before dropping near the symmetrical incoherent tilt grain boundary. Which further results in the consistency of motion mechanism within the boundary set.

[110]			
Σ	θ	GB Plane	CSL
3	70.53	$(\bar{1}11)$ $(1\bar{1}2)$ $(110)*$	$\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 2 & 0 \end{pmatrix}$

Figure 6: [110] Tilt Axis

Due to the various properties of <110> Σ3 is more thermal activated it has high mobility angle which provides us the structuring of the motion mechanism and mechanical utilities.

3.3 Grain boundaries structure file

To run the stimulation, we require the prior grain boundary file which available to us, the script of that data file should be saved in name of Fe_110_sig3.txt and Fe_110_sig3.in, where sigma3 describe a three-dimensional coincidence site lattice (CSL). The coincidence lattice is generated by rotation around <110> axis by 70.5 degree i.e. let[1-11] lattice site in one crystal to coincident with [1 1 -1] lattice site in another lattice. As for the boundary plane, sigma 3 does not tell you about the actual boundary plane, but it tells one what are the potential grain boundaries with high CSL sites, i.e. the interface prefers to pass high density of coincidence site in order to lower the boundary energy. According to the CSL lattice on (110) plane(see attached figure, red points = lattice in crystal 1, blue = crystal 2, green points are coincidence lattice site), the possible "symmetric tilt grain boundary" is (1 -1 2) with highest CSL density or (1-1-1) with second highest CSL density. Therefore, the formal description should be like Σ3(1-1-1)[110] symmetric tilt grain boundary, Σ3(1-12)[110] symmetric tilt grain boundary.

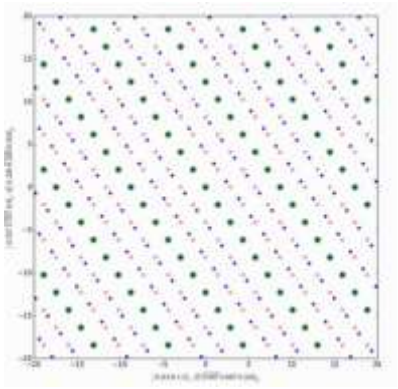

Figure 7: Grain boundary Fe_110_sig3

The above image shows the visualized form of the Fe_110_sig3 grain boundary structure file. This will be used our data file of grain boundary in LAMMPS to perform the stimulation upon it until the fracture is obtained. For this we have used the 600 atoms of Fe with grain boundary at tilt axis <110> and Σ3 with rotation 70.5 degree.

3.4 LAMMPS Input script

To run the stimulation, we need an input script which provides the command to the LAMMPS to perform each step of the stimulation. The question arises that what actually this input script contains? Well the clear answer is that it provides basic fundamentals of stimulation require to perform. Although we need to ensure that input script should be saved into the .in format, to make LAMMPS to read it as input file.

Our main objective is to develop a stress-strain relation of iron grain boundary under fracture and perform the metrics analyses which will provide per-atom properties. The script needs the grain boundary file to perform the stimulation which is fed to the variable datfile. The variable nloop defines how many times the strain will be increased and the number of points stress is calculated. Other variables as the strain increment and the number of replications has been written into the input script. Before strain is applied to the atoms those atoms are far from the grain boundary (as defined by datfile) are deleted to prevent the unwanted transition between the periodic boundaries and to decrease the stimulation time. Then two smaller groups of atoms (defined by deldist and fixdist) are being of forced to value zero. These two fixed groups are incrementally displaced to generate strain value until the fracture. The interatomic potential needed for the stimulation to run is Hepburn and Auckland (2008) Fe-C. Particularly this interatomic potential is used to create the grain boundaries studies of segregation of C atoms to various positions and different grain boundaries, although C part of potential is not used.

Figure 8: Initial visuals of the simulations.

From the above figure we can clearly see that stimulation box is not full with atoms as earlier discussed that some unwanted atoms have been deleted in order to prevent the interference in periodic boundary of the stimulation cell. Generally, there are 600 atoms were created from datfile now fixing the variables it has come all the way to only 240 atoms. On these remaining atoms the stress-strain relationship will be conducted under the fracture conditions.

3.5 Per-atom metrics

After stimulation is done now, we will conduct the per atom metrics analyse. With the help of the Molecular Dynamics stimulation we can check per atom properties from our stimulation cells. There are some steps that LAMMPS will go through it: -

- First it will upload the datfile which is also known as the grain boundary file. It will read all the data of atom positions and grain boundaries energies.
- Then we need a interatomic potential i.e. Hepburn and Auckland 2008 Fe-C which will provide the segregation of C atoms at different positions of grain boundary.
- Now we need to define some atoms randomly from the stimulation cell to get the per atom properties.
- Now it will run short minimization of dump file that includes the compute atoms it is necessary to initialize the stimulation.
- Then stimulation will loop over those atoms for 150 times.
- Providing LAMMPS a command to print those atom metrics from log file along with flag, it is important when we mine the per atom metrics from log file.
- Then this delete all the dump files that were created earlier when we developed the grain boundary fracture and stress-strain relationship.

3.6 Visualization

After all the stimulation is done now, we will visualize the processes that we performed in the LAMMPS. To visualize the stimulations, we will use different tools that are capable to read those files as a syntax. For movie and pictorial format OVITO is our best tool, it allows us to see the stimulation on screen. The OVITO will load all the dump files that are in format of .cfg and visualize the stimulation.

For graphical and graphical mapping image-based visualization we will use python. Python helps us to map out the large and complex data that has develop during stimulation and provide the graphical interpretation to us. Also, python will import data from the LAMMPS log file which is known as our output file. Here are the python codes used for visualization.

3.6.1 Stress-strain relationship and Per Atom Metrics.

From the python codes we will get the pop ups of graph and image mapping of atom using the data created from the LAMMPS. This will provide the end results of the stimulation which helps to analyse and investigates the grain boundary properties in different conditions with different positions.

Results

The following images have been visualised by the OVITO software at different loops depicting the progress of fracture in tilt grain boundary.

(a)

(b)

(c)

Figure 9: a) Left Side view at step 1; b) Top view at step 1; c) isometric view at step 1

It is observed from the above images that the atoms have been setup in the stimulation cell at initialization also the extra atoms in this stimulation are been deleted with the help of potential file to avoid the interference in the periodic boundary of the stimulation cell. According to the data file the initial number of atoms were 600 but while setting up the stimulation only 240 atoms were left in the stimulation box.

(a)

(b)

(c)

Figure 10: a) Left view at step 144; b) Top view at step 144; c) Isometric view at step 144

From the pictorial representation of the stimulation shown above, the fracture has finally obtained at step 144.

Figure 11: Left side view at step 150

At the final step of the stimulation the atoms were pulled back such that they were dislocated from their original position. This will create the end result i.e. Fe symmetrical tilt grain boundary under fracture.

As stated above in the report, the stress-strain relationship based on the preceding datafile "data.Fe_110_sig3_fracture.txt" which investigates and stores strain information in the first column while stress tensor information in the second through seventh columns, and stores the total potential energy of the cell in the eight column is also obtained. As per the ‘nloop’ variable the simulation should have looped 150 times, so there should be 150 entries which end at a strain of 0.15 along with the initial entry of stress and strain at zero.

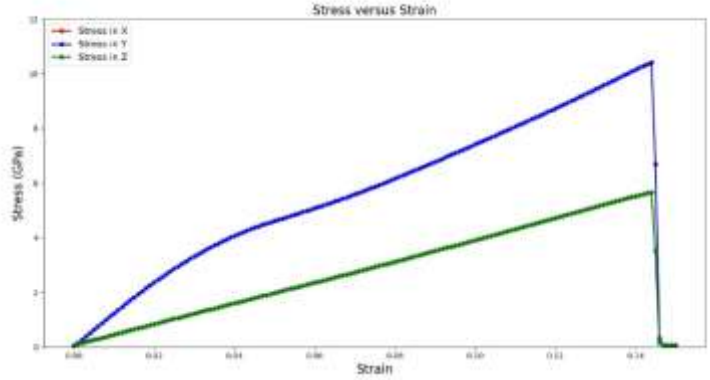

Figure 12: Stress – Strain Graph

Notice that as the strain in the y-direction is applied the stress in y is increasing, but at the same time stress in the x- and z-directions are also increasing. This is occurring due to our constraint of fixing the simulation cell which are bounded in the x- and z- directions. Hence if allowed to relax the simulation cell in the directions of x and z axis as we are straining the configuration, it would likely take longer time to fracture.

According to the data, it can be used for different number of things. Like just plotting the atomic coordinates, coloured by the in-plane coordinate (z-direction). Hence using the colourmap to give the classic black and white grain boundary structure look for atoms that sit on different {110} planes. We added a second set of atoms in the x-direction to extend the simulation cell (replicate atoms because of the periodic boundary) and only chose those atoms within 5 Angstroms of the grain boundary.

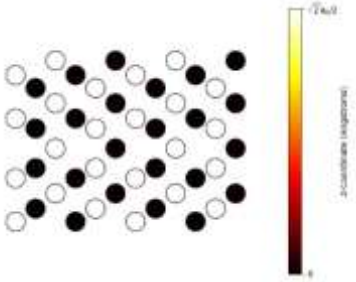

Figure 13: Colour Map within the 5 Angstrom of grain boundary.

2.019 value is selected for the tick mark on the colour bar by looking at the minimum and maximum z-coordinates for the dataset (even the grain boundary atoms stayed in the {110} planes). Knowing that it is a BCC crystal structure in the <110> direction, there is a $\sqrt{2}/2$ spacing between {110} planes. So, the lattice constant for this interatomic potential must be: lattice constant, a_0 =2.855113245669044 Angstroms.

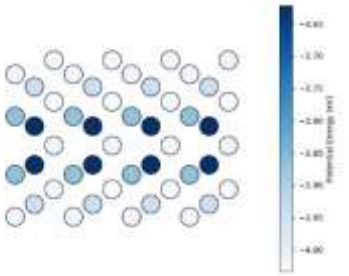

Figure 14: Potential Energy of each atom.

The potential energy of each atom can be seen by the above picture. It is observed that the potential energy is maximum of the atoms along the centre line and it goes on decreasing as we move away from it. The value of maximum potential energy observed was -3.65 eV while minimum is -4.0 eV.

CONCLUSION

From the above analysis and investigation, we can conclude that grain boundary creates necessary hinderance in order to enhance the material properties. It is majorly dependent on the tilt axis of the grain boundary and the value of Σ which is the coincidence ratio. The time required to fracture can be extended by relaxing the stimulation cell in the direction of x and z-axis that may lead to improvement in the resistance to fracture of the material. Even though having the Tilt grain boundary <110> tilt axis at Σ value 3 has shown enhancement in various mechanical properties which can be further used in different industrial applications. After analysing the data, we observed that the spacing between the {110} planes is $\sqrt{2}/2$. Also viewed from the colour map at Z- axis lead to increment of potential energy at the atoms near to the central axis. This shows us that the grain boundary at the certain tilt axis has shown the possessive nature towards the mechanical properties which beneficial for commercial usability.

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