Correlation between misorientations and stored energy gradients during elastic deformation at grain boundaries

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Abstract

Correlation study of energy gradient and misorientation angle at the grain boundaries gives us deep insight on the behaviour of materials during deformation. Thus, it warrants for experimental and computational research to further understand the relation between these properties. In this work, we have used finite element analysis via Abaqus to simulate elastic deformation of polycrystals and calculate the distributions in stored energy. We then found the correlation between the misorientations and stored energy gradients at the grain boundaries. We utilized DREAM.3D for polycrystal generation.

Keywords: Grain boundary Engineering, finite element analysis, Abaqus, energy gradients, elastic deformation, correlation

1. Introduction

Crystalline materials exhibit long and short range order. By the virtue of solidification and processing of metals and alloys, crystallites of differing orientations impinge upon one another. This results in a defect called grain boundary. Thus, a grain boundary is an interface between two or more grains. Over the years, many models have been proposed to explain the structure and properties of grain boundaries. The parameters usually studied with respect to the grain boundaries are the misorientation and its relation with other properties. Based on the misorientation angle, low angle grain boundaries(LAGB) with misorientation $< 15^o$ are explained using lattice distortion model and high angle grain boundaries(HAGB) with misorientation $> 15^o$ are explained using

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coincident site lattice theory.

In order to completely characterize a grain boundary, five independent parameters are necessary. The misorientation between adjacent grains can be quantified by the three Euler angles which are operated on grain A to generate grain B. The grain boundary plane is positioned using two more parameters in the form of miller indices {hkl}.

Deformation is the process of changing the shape or size of a given material by applying a force or by a change in temperature. Depending on the type of material, size and geometry of the object, and the forces applied, different types of deformation take *place*[1].

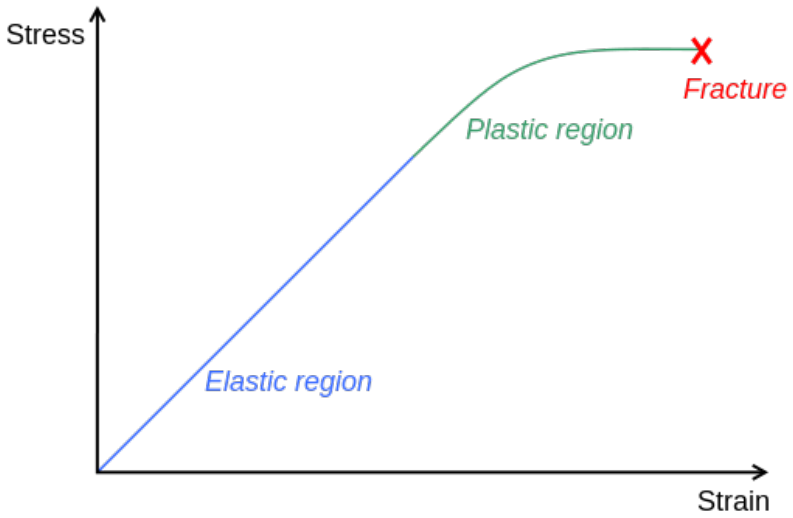


Figure 1: Stress Strain curve for a ductile *metal*[1]

The aim of this work is to use finite element analysis with *Abaqus*[2] to deform the equiaxed cubic polycrystal. The polycrystal is generated using *DREAM.3D*[3]. In this work, we deform the material elastically. We calculate the stored energy at the deformed *state*[1]. We then find the misorientations between grains in our equiaxed cubic polycrystal and their correlation with the energy gradients across grain boundaries. As an assumption, we have not accounted for the symmetry found in a cubic crystal during the calculation of misorientation angles. Our work is based on the elastic properties of copper. The material is defined by 27000 element cube (30 elements a side). We also observed the relation between the number of unique grain boundaries present as the number of elements grows.

$$Energy = \sigma_{ij}\epsilon_{ij} * Volume \tag{1}$$

Element	C_{1111}	C_{1122}	C_{1212}
Copper	168000	121400	75400

Table 1: Elastic properties of copper utilized

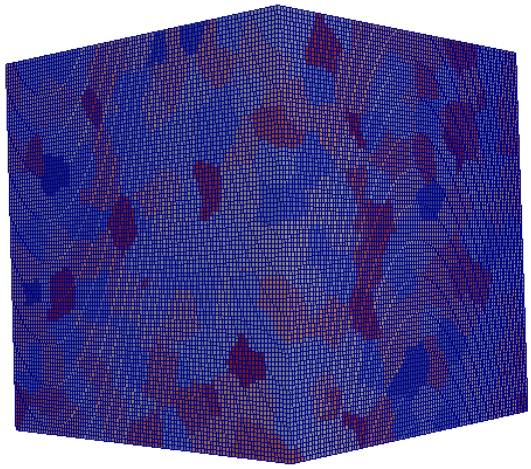


Figure 2: One of the 3D polycrystals *developed*[3][4]

2. Materials & Methods

We utilized DREAM.3D to generate multiple polycrystals and assigned the grains orientation randomly. The grains are of the default size defined in the stats generator in DREAM.3D. We utilized Abaqus to implement elastic deformation and obtain the required parameters to calculated the energy of each *element*[1]. We utilized scripts developed in *Matlab*[5] and *R*[6][7] to find the correlation between the misorientation and the elastic energy gradients at the grain boundaries as well as visualize the results. The elastic properties utilized are present in Table 1

3. Calculations

In this work, we used equation 1 to find the elastic energy of each integration point in each element. We then averaged the energy over the volume of the integration $points^2$.

$$Energy_{element} = \frac{\Sigma_{i=1}^{IP} Energy_i}{\Sigma_{i=1}^{IP} Volume_i} \tag{2}$$

where IP is the number of integration points.

We defined a grain boundary if two elements shared 4 $nodes^3$.

$$n(Nodes_{element1} \cap Nodes_{element2}) = 4 \tag{3}$$

The energy gradient across the grain boundary is the difference between the energies of the two elements.

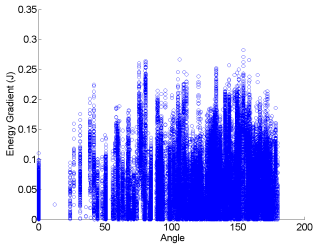
To find the misorientation angle between two elements, we converted the euler angles to a matrix $notation^{[8]}$. We find the rotation matrix and find the misorientation angle from the rotation matrix.

4. Results

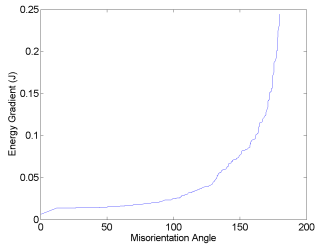
In this work, we have obtained the correlation for 5 randomly generated polycrystals. Sample 1 is a pre-generated crystal utilized for comparison with the other generated crystals. We also averaged the energy at each misoirentation angle to see the difference in the correlation. We did not apply the symmetry corresponding to to the cubic crystal. Hence the misorientation angle ranges from 0 to 180^o. We also observed the variation in grain boundaries based on the number of grains before and after averaging.

$$Energy_{Avg}(\theta) = \frac{\Sigma_{i=1}^{K} Energy_i(\theta)}{K} \tag{4}$$

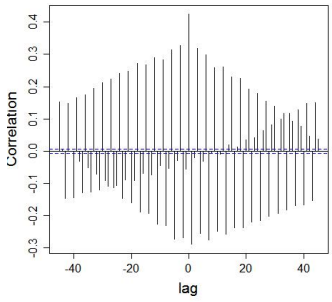
4.1. Sample 1



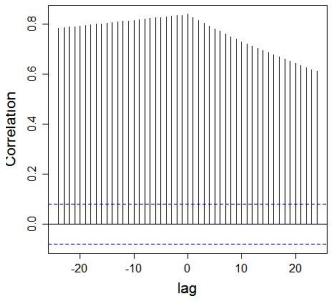
(a) Energy gradient vs Misorientation Plot before averaging over misorientation



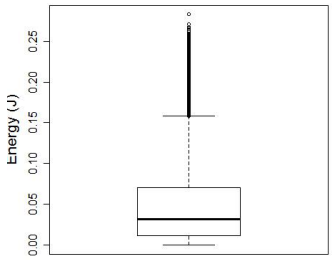
(b) Energy gradient vs Misorientation Plot after averaging over misorientation



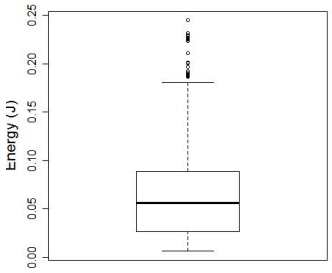
(c) Correlation between Energy gradient and Misorientation before averaging



(d) Correlation between Energy gradient and Misorientation after averaging



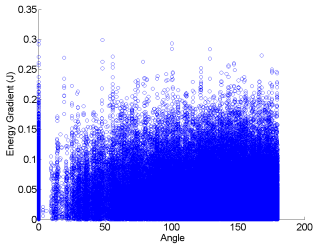
(e) Box plot of energy gradient before averaging



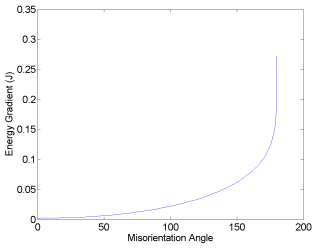
(f) Box plot of energy gradient after averaging

Figure 3: Relation between energy gradient and misorientation for Sample 1

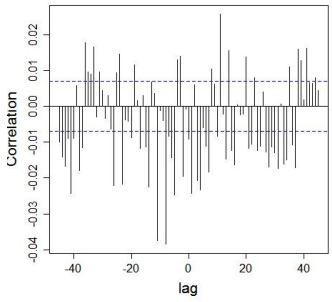
4.2. Sample 2



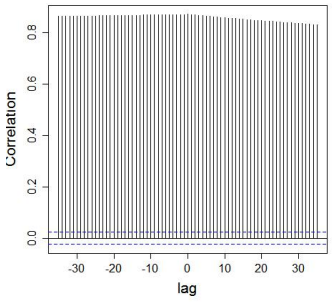
(a) Energy gradient vs Misorientation Plot before averaging over misorientation



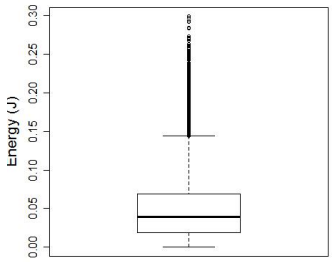
(b) Energy gradient vs Misorientation Plot after averaging over misorientation



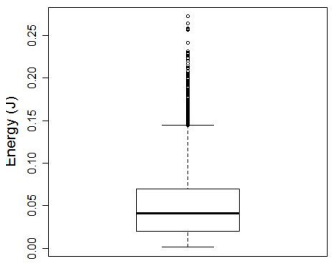
(c) Correlation between Energy gradient and Misorientation before averaging



(d) Correlation between Energy gradient and Misorientation after averaging



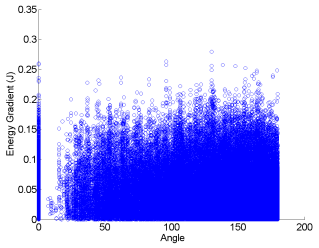
(e) Box plot of energy gradient before averaging



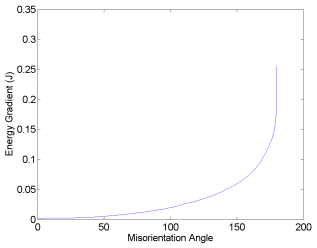
(f) Box plot of energy gradient after averaging

Figure 4: Relation between energy gradient and misorientation for Sample 2

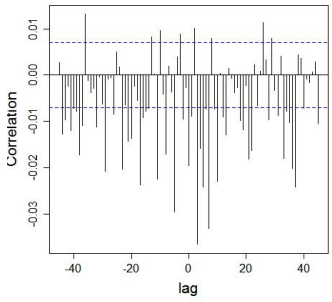
4.3. Sample 3



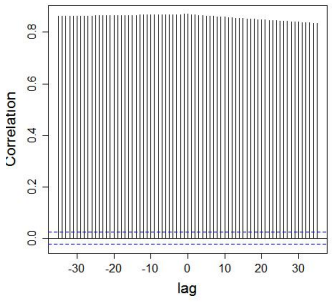
(a) Energy gradient vs Misorientation Plot before averaging over misorientation



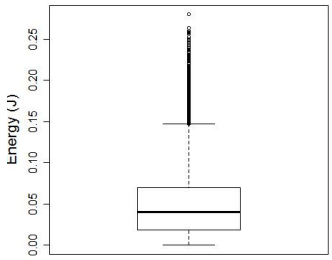
(b) Energy gradient vs Misorientation Plot after averaging over misorientation



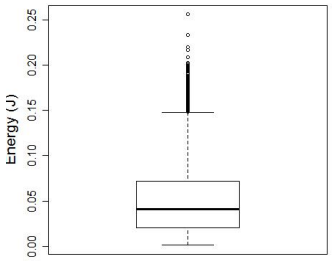
(c) Correlation between Energy gradient and Misorientation before averaging



(d) Correlation between Energy gradient and Misorientation after averaging



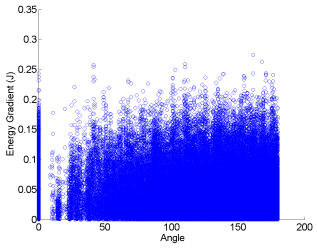
(e) Box plot of energy gradient before averaging



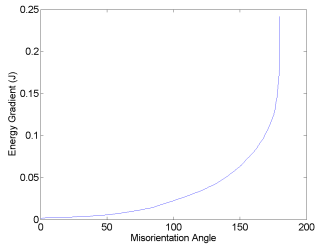
(f) Box plot of energy gradient after averaging

Figure 5: Relation between energy gradient and misorientation for Sample 3

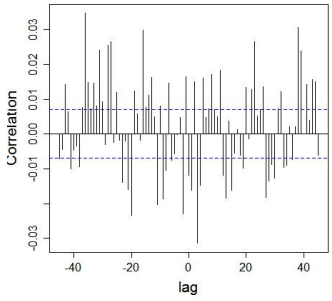
4.4. Sample 4



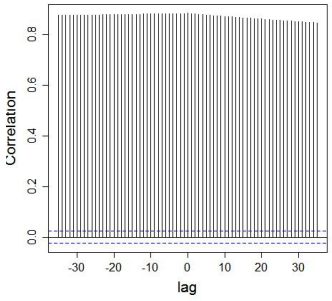
(a) Energy gradient vs Misorientation Plot before averaging over misorientation



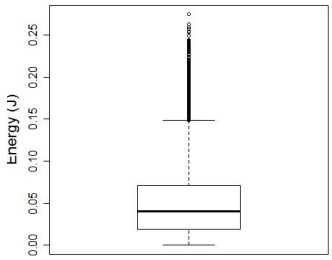
(b) Energy gradient vs Misorientation Plot after averaging over misorientation



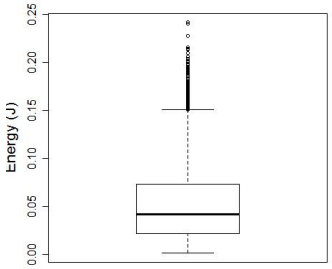
(c) Correlation between Energy gradient and Misorientation before averaging



(d) Correlation between Energy gradient and Misorientation after averaging



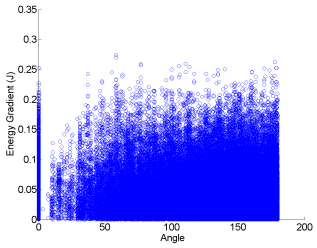
(e) Box plot of energy gradient before averaging



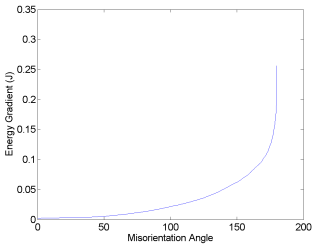
(f) Box plot of energy gradient after averaging

Figure 6: Relation between energy gradient and misorientation for Sample 4

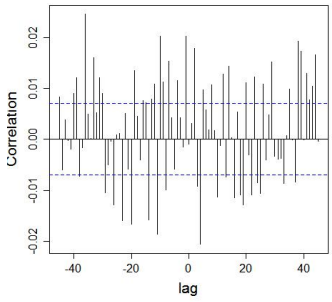
4.5. Sample 5



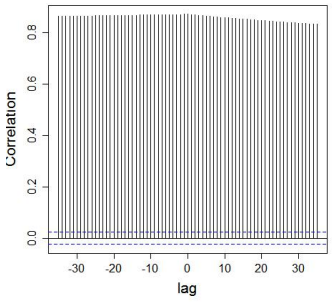
(a) Energy gradient vs Misorientation Plot before averaging over misorientation



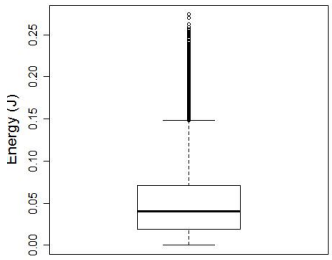
(b) Energy gradient vs Misorientation Plot after averaging over misorientation



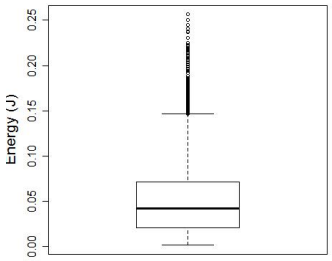
(c) Correlation between Energy gradient and Misorientation before averaging



(d) Correlation between Energy gradient and Misorientation after averaging



(e) Box plot of energy gradient before averaging



(f) Box plot of energy gradient after averaging

Figure 7: Relation between energy gradient and misorientation for Sample 5

Sample	Correlation before averaging	Correlation after averaging	Curve fit post averaging (y - Energy (J), x - radians)
Sample 1	0.424	0.839	$y = e^{(0.3504x^2 - 0.2671x - 4.274)}$
Sample 2	0.009	0.872	$y = e^{(1.308x - 6.139)}$
Sample 3	0.019	0.869	$y = e^{(1.384x - 6.371)}$
Sample 4	0.012	0.884	$y = e^{(1.354x - 6.249)}$
Sample 5	0.001	0.871	$y = e^{(1.365x - 6.294)}$

Table 2: Correlation between energy and misorientation before and after averaging

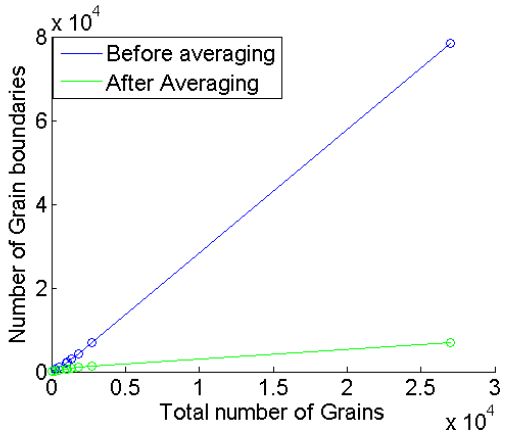


Figure 8: Number of grain boundaries before and after averaging as number of grains increases

5. Discussion

From the results, we can deduce that all samples show similar correlation between the energy and misorientation as seen in Figs. 3 4 5 6 7. While the correlation before averaging is negligible, the correlation post averaging is very high. By averaging we remove much of the noise present in the energy at every misorientation angle and hence this improves the correlation. We see that energy increases exponentially as the misorientation increases as seen in Table 2.

6. Conclusions

In this work, we generated multiple randomly oriented polycrystals which have equiaxed grains and observed the correlation between the misorientation and the stored energy gradients due to elastic deformation across the grain boundaries. We observed the correlation before and after averaging the energy gradient at every misorientation. We also fit an exponential equation to show the relation between misorientation and energy gradients post averaging.

Future work in this direction would be to incorporate the symmetry seen in cubic materials and see how this affects the correlation. The current work has been pursued for copper. Similar studies can be done for other elements. We could also see the difference between equiaxed and rolled grains as well as other crystal structures.

7. Acknowledgements

We would like thank Aditya Lakshmanan and Chaitanya P for their contributions towards this project. We would like to thank Dr. G. Phanikumar for the facilities of his group. We would like to thank IIT Madras for providing us access to their computational facilities. We thank the Metallurgical and Materials Engineering Department for giving us this opportunity to pursue this work.

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