Stability of Junctions in Grain Networks

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July 2015

Abstract

Misorientation of grains in polycrystalline materials results in the formation of grain boundaries. Materials composed of many grains will cause the formation of a large network of boundaries. The physical forces acting on these boundaries results in an interface energy which determines the stability of the grain boundary networks. In two dimensional thin films, it is well known that three boundaries meeting at a point, forming a triple junction, is stable. The goal of this paper is to determine the potential for stability of higher m-junctions of grain boundaries. Using the Read-Shockley model for grain boundary energy, we prove that many 4-junctions cannot be stable, and conjecture that under the Read-Shockley model no stable 4-junctions can exist. However, when considering other possible models that share qualitative properties with the Read-Shockley model, we find that it is possible for many different 4-junctions to be stable.

1 Introduction

Polycrystalline materials contain highly ordered arrangements of atoms or molecules known as grains. Each grain contains of a perfect crystalline structure. When grains with different crystallographic orientations meet they form an interface known as a grain boundary [2]. Differences in grain orientation can result in changes of important physical properties, including thermal and electrical conductivity as well as fracture strength.

The angles at which multiple grain boundaries meet and the relationship between the lattice structures of adjacent grains effect the physical forces acting on these boundaries. Under certain conditions, such as the heating of a polycrystalline materials, grains will seek a more preferable configuration by converting and absorbing parts of the lattice structures of their neighbors in a process called grain growth [6].

We will be investigating the stability of junctions in two-dimensions. In a system with equal interface energies between adjacent grains, it is well know that the triple junction with straight boundaries 120° apart is minimizing [3]. This research is considering the possibility of higher junctions in systems with unequal interface energies.

2 Motivation

Polycrystalline materials include many common metals and ceramics. Material scientists, engineers, and applied mathematicians often seek to create accurate simulations attempting to depict grain growth in polycrystalline materials, as accurate simulations can provide better tools for scientific observation and industrial production of these materials.

When creating simulations, certain assumptions about the physical properties must be made. More accurate assumptions lead to more accurate simulations.

Although it is well known that 3-junctions are minimizing in a system with equal interface energies, the possibility of stability of higher m-junctions in a system with unequal interface energies is unknown. Knowing if the existence of a stable m-junction is possible will allow for more accurate assumptions to be made when creating computer simulations of grain growth.

3 Model for Grain Boundary Energy

Grain boundaries have been extensively studied and modeled by material scientists. One of the most well known of which is the Read-Shockely model [7], which models the energy of the grain boundary between the grains of two different materials:

$$E = E_0\theta[A - \ln\theta] \tag{1}$$

Where E_0 and A depend on the physical properties of the materials, including shear modulus and Poisson's ratio.

This model is most accurate for low-angle boundaries, and has been further expanded on by Brandon [1], who noted a saturation at high-angle boundaries. Furthermore, when studying boundaries of only one material in 2-dimensions, (1) can be simplified. Combining these models, we get

$$E(\theta) = \begin{cases} \frac{\theta}{B}\left(1 - \log\left(\frac{\theta}{B}\right)\right) & \text{if } \theta < B \\ 1 & \text{if } B \leq \theta \leq \pi/2 - B \\ \frac{\pi/2-\theta}{B}\left(1 - \log\left(\frac{\pi/2-\theta}{B}\right)\right) & \text{if } \pi/2 - B < \theta \end{cases} \tag{2}$$

Where θ is the angle between the lattice structures of the grains, and $0 < B \leq \pi/4$

4 Methods of Studying Stability

There are many different ways to study the stability of systems. The two methods used in this research are the Lawlor and Morgan's Calibration Method [5] and the Herring angle condition [4]

4.1 Calibration Method

From [5], the Immiscible Fluids Theorem II tells us that given interface energies $\sigma_{i,j} = \sigma_{j,i} > 0$ for $1 \le i \ne j \le m$, a hypersurface $C \subset B(0,1) \subset \mathbb{R}^n$, which divides $B(0,1)$ into regions $\Sigma_1, \dots, \Sigma_m$ separated by hyperplanes $H_{i,j}$ oriented with unit normals $n_{i,j} = -n_{j,i}$ pointing from Σ_i to Σ_j, is minimizing if:

Whenever k hyperplane pieces $H_{i_1,i_2}, H_{i_2,i_3}, \dots, H_{i_1,i_k}$ meet along a co-dimension-2 plane,

$$\sigma_{i_1,i_2} n_{i_1,i_2} + \cdots + \sigma_{i_k,i_1} n_{i_k,i_1} = 0 \tag{3}$$

And, for any distinct integers $1 \le i_1, \dots, i_s \le m$ where $H_{i_J,i_J+1} \ne \emptyset$,

$$|\sigma_{i_1,i_2} n_{i_1,i_2} + \cdots + \sigma_{i_{s-1},i_s} n_{i_{s-1},i_s}| \le \sigma_{i_1,i_s} \tag{4}$$

4.2 Herring Angle

Consider three adjacent regions $\Sigma_{i-1}, \Sigma_i, \Sigma_{i+1}$ separated by hyperplanes $H_{i-1,i}$ and $H_{i,i+1}$, initially the angle α_i apart. Suppose the configuration becomes perturbed in such a way as that a hyperplane $H_{i-1,i+1}$ forms between Σ_{i-1} and Σ_{i+1} and creates a triple junction with $H_{i-1,i}$ and $H_{i,i+1}$. Let the angle between $H_{i-1,i+1}$, $H_{i-1,i}$ be denoted as $Herr(i-1,i,i+1) = Herr(i-1,i+1,i)$; the angle between $H_{i-1,i}$,$H_{i,i+1}$ as $Herr(i,i-1,i+1) = Herr(i,i+1,i-1)$; and the angle between $H_{i,i+1}$,$H_{i-1,i+1}$ as $Herr(i+1,i,i-1) = Herr(i+1,i-1,i)$.

The Herring Angle Condition states that

$$\frac{\sin(Herr(i,i-1,i+1))}{\sigma_{i-1,i+1}} = \frac{\sin(Herr(i-1,i,i+1))}{\sigma_{i,i+1}} = \frac{\sin(Herr(i+1,i,i-1))}{\sigma_{i,i-1}} \tag{5}$$

and the configuration is unstable if, for any $1 \le i \le m$, $Herr(i,i-1,i+1) > \alpha_i$

4.3 Equivalence

Note that the both the Calibration Method and the Herring Angle condition are conditional statements. Thus, the Calibration Method cannot prove instability, and the Herring Method cannot prove stability. However, for $C \subset B(0,1) \subset \mathbb{R}^2$ where $H_{i,i+1(\mathrm{mod}/m)} \ne \emptyset$ and all other $H_{i,j} = \emptyset$, the statements become biconditional for $m = 4$.

Using polar coordinates and the law of cosines, the herring angles for any two adjacent hyperplanes can be given as:

$$Herr(i-1,i,i+1) = \arccos \frac{r - \cos(\phi)}{\sqrt{r^2 - 2r\cos(\phi) + 1}} \tag{6}$$

$$Herr(i+1,i,i-1) = \arccos \frac{r - \cos(\phi - \alpha)}{\sqrt{r^2 - 2r\cos(\phi - \alpha) + 1}} \tag{7}$$

$$
\begin{aligned}
Herr(i,i+1,i-1) &= 2\pi - (Herr(i+1,i,i-1) + Herr(i-1,i,i+1)) \\
&= \arccos \frac{\cos\alpha + r^2 - r\cos(\phi) - r\cos(\phi-\alpha)}{\sqrt{(r^2-2r\cos(\phi)+1)(r^2-2r\cos(\phi-\alpha)+1)}} \qquad (8)
\end{aligned}
$$

Where ϕ is the angle of perturbation and α is the initial angle between $H_{i-1,i}$ and $H_{i,i+1}$.

With the trigonometric identity $\sin(\arccos(x)) = \sqrt{1-x^2}$, it follows from (5) that:

$$
\frac{\sqrt{1-\frac{(\cos\alpha+r^2-r\cos(\phi)-r\cos(\phi-\alpha))^2}{(r^2-2r\cos(\phi)+1)(r^2-2r\cos(\phi-\alpha)+1)}}}{\sigma_{i+1,i-1}} = \frac{\sqrt{\frac{1-\cos^2(\phi)}{r^2-2r\cos(\phi)+1}}}{\sigma_{i,i+1}} = \frac{\sqrt{\frac{1-\cos^2(\phi-\alpha)}{r^2-2r\cos(\phi-\alpha)+1}}}{\sigma_{i,i-1}}
$$

which becomes:

$$
\frac{(r^2-2r\cos(\phi)+1)(r^2-2r\cos(\phi-\alpha)+1)-(\cos\alpha+r^2-r\cos(\phi)-r\cos(\phi-\alpha))^2}{\sigma^2_{i+1,i-1}}
$$

$$
= \frac{(1-\cos^2(\phi))(r^2-2r\cos(\phi-\alpha)+1)}{\sigma^2_{i,i+1}} = \frac{(1-\cos^2(\phi-\alpha))(r^2-2r\cos(\phi)+1)}{\sigma^2_{i,i-1}}
$$

From this, we can also see that

$$
\frac{\sigma_{i,i+1}}{\sigma_{i,i-1}} = \frac{\sin(\phi)}{\sin(\phi-\alpha)}\sqrt{\frac{r^2-2r\cos(\phi-\alpha)+1}{r^2-2r\cos(\phi)+1}}
$$

Thus, near the origin the angle of perturbation is determined by

$$
\phi = \arctan \frac{\sigma_{i,i+1}\sin(\alpha)}{\sigma_{i,i+1}\cos(\alpha)+\sigma_{i,i-1}} \qquad (9)
$$

Inserting this back into (5):

$$
\frac{\sin(\arctan \frac{\sigma_{i,i+1}\sin(\alpha)}{\sigma_{i,i+1}\cos(\alpha)+\sigma_{i,i-1}})}{\sigma_{i,i+1}} = \frac{\sin(\arctan(\frac{\sigma_{i,i+1}\sin(\alpha)}{\sigma_{i,i+1}\cos(\alpha)+\sigma_{i,i-1}})-\alpha)}{\sigma_{i,i-1}} = \frac{\sin(\alpha)}{\sigma_{i+1,i-1}}
$$

Then, from the trigonometric identity $\sin(\arctan(x)) = x/\sqrt{1+x^2}$,

$$\frac{\sin(\alpha)}{\sigma_{i+1,i-1}} = \frac{\sin\alpha}{\sqrt{\sigma_{i,i+1}^2 + 2\sigma_{i,i+1}\sigma_{i,i-1}\cos(\alpha) + \sigma_{i,i-1}^2}}$$

Thus, the configuration is unstable by the Herring Angle Condition if

$$\sqrt{\sigma_{i,i+1}^2 + 2\sigma_{i,i+1}\sigma_{i,i-1}\cos(\alpha) + \sigma_{i,i-1}^2} > \sigma_{i+1,i-1} \tag{10}$$

Therefore, (10) and (4) are biconditional when $m = 4$, $H_{i,i+1(\text{mod}/m)} \neq \emptyset$, and all other $H_{i,j} = \emptyset$

5 Stability of 4-junctions in Grain Networks

5.1 Read-Shockley Model

Consider a grain network which divides $B(0,1)$ into grains $\Sigma_1, \ldots, \Sigma_4$ separated by boundaries $H_{i,j}$ extending from the origin. Each grain has an angle of lattice structure $0 \leq \theta_i \leq \pi/2$ and each grain boundary $H_{i,j}$ has an interface energy $\sigma_{i,j} = E(\theta_{i,j})$ where E is the function given by (2) and $\theta_{i,j} := |\theta_i - \theta_j|(\text{mod } \pi/2)$

Furthermore,

$$\sum_{i=1}^{4} \alpha_i = 2\pi$$

and

$$\sum_{i=1}^{4} \theta_{i,i+1(\text{mod } 4)} = \pi/2$$

As shown in the last section, this configuration will be minimizing if and only if (3) and (4) are true. Thus, this configuration is stable when

$$\sigma_{1,2}n_{1,2} + \sigma_{2,3}n_{2,3} + \sigma_{3,4}n_{3,4} + \sigma_{4,1}n_{4,1} = 0 \tag{11}$$

$$|\sigma_{1,2}n_{1,2} + \sigma_{2,3}n_{2,3}|, |\sigma_{4,1}n_{4,1} + \sigma_{3,4}n_{3,4}| \leq \sigma_{1,3} \tag{12}$$

and

$$|\sigma_{2,3}n_{2,3} + \sigma_{3,4}n_{3,4}|, |\sigma_{1,2}n_{1,2} + \sigma_{4,1}n_{4,1}| \leq \sigma_{2,4} \tag{13}$$

Consider a 4-junction with 4 equal partitions and $\sigma_{1,2} = \sigma_{2,3} = \sigma_{3,4} = \sigma_{4,1}$. This implies $\theta_{1,2} = \theta_{2,3} = \theta_{3,4} = \theta_{4,1} = \pi/8$. These values will be minimized when $B = \pi/4$. Thus, their minimum is $.5(1 - \ln .5) \approx .8466$. It also follows that $\theta_{1,3} = \theta_{2,4} = \pi/4$, therefore $\sigma_{1,3} = \sigma_{2,4} = 1$. It is clear that this configuration fulfills (11). However, this fails to fulfill (4). Furthermore, notice that rotation of any $H_{i,j}$ will result in an increase in the left side of either (12) or (13). Therefore, for equal $\sigma_{i,i+1}$, no configuration can be stable with Read-Shockley.

Consider a 4-junction with $\theta_{1,2} = \theta_{3,4}$ and $\theta_{2,3} = \theta_{4,1}$ This implies $\theta_{1,3} = \theta_{2,4} = \pi/4$, therefore $\sigma_{1,3} = \sigma_{2,4} = 1$. These values will be minimized when $B = \pi/4$. When all partitions are equal, it is clear that this configuration fulfills (11). As $\theta_{1,2}$ approaches 0, the left side of (12) and (13) will approach 1, but will always be greater than 1. Again, rotating any boundary will cause one of the left sides of (12) or (13) to increase, so it can never be stable.

We conjecture that no 4-junction can be stable with the Read-Shockley model. It may be possible to prove this by finding a function which, for all possible $\theta_{i,j}$, provides $\alpha_1, \ldots, \alpha_4$ such that (11) is true but all inequalities in (12) and (13) are false.

5.2 Other Models

The Read-Shockley model is not always accurate. The qualitative requirements for the Read-Shockley model $E(\theta)$ in $\mathbb{R}^2$ are:

$E(0) = 0$

$E(\theta > 0) > 0$

$E' > 0$

$E'' < 0$

$E(\theta)$ reflects over the line $\theta = \pi/4$

With these qualitative requirements, many other possible models allow for the formation of stable 4-junctions. For example, consider the Read-Shockley equation where the natural logarithm is replaced with the base 10 logarithm. In this model, $E(\pi/8) = k \approx .6505$. Thus, for a 4-junction with 4 equal partitions (11) becomes

$$k(-1,0) + k(0,-1) + k(1,0) + k(0,1) = 0$$

and (12) and (13) become

$$\sqrt{2k^2} \approx .92 \leq 1$$

It is clear that both of these are true. Thus, under this model the 4-junction is stable.

6 Conclusion

The calibration method was found to be biconditional under specific conditions for the problems investigated in this research. By applying this, it was shown that using the Read-Shockley model for grain boundary energy, there cannot be any stable 4-junction with $\theta_{1,2} = \theta_{2,3} = \theta_{3,4} = \theta_{4,1} = \pi/8$ or $\theta_{1,2} = \theta_{3,4}$ and$\theta_{2,3} = \theta_{4,1}$. Based on these results, we conjecture that in the Read-Shockley model all possible 4-junctions regardless of Brandon Angle, angles between grain boundaries, and angles between lattice structures of the grains, will be unstable. However, when considering other models, many different junctions can be stable.

7 Acknowledgments

The author would like to thank Selim Esedoḡlu for guidance and support in this research, and the University of Michigan for the opportunities given by its REU program. The author was supported by NSF DMS-1317730.

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