LARGE TIME ASYMPTOTIC BEHAVIOR OF GRAIN BOUNDARIES MOTION WITH DYNAMIC LATTICE MISORIENTATIONS AND WITH TRIPLE JUNCTIONS DRAG

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Abstract. Most technologically useful materials are polycrystalline microstructures composed of a myriad of small monocrystalline grains separated by grain boundaries. Dynamics of grain boundaries play an essential role in defining the materials properties across multiple scales. In this work, we study the large time asymptotic behavior of the model for the motion of grain boundaries with the dynamic lattice misorientations and the triple junctions drag.

1. Introduction

Most technologically useful materials are polycrystalline microstructures composed of a myriad of small monocrystalline grains separated by grain boundaries. Dynamics of grain boundaries play an essential role in defining the materials properties across multiple scales. Experimental and computational studies provide large amounts of information about both geometric features and crystallography of the grain boundary network in material microstructures.

The focus of this work is on the dynamics of a planar grain boundary network. A classical model for the motion of grain boundaries in polycrystalline materials is due to Mullins and Herring [18, 29, 30]. The model is based on the assumption of the motion by mean curvature as the local evolution law for the grain boundaries. Furthermore, under the assumption that the total grain boundary energy depends only on the surface tension of the grain boundaries, the motion by mean curvature is consistent with the dissipation principle for the total energy. In addition, to have a well-posed model for the evolution of the grain boundary network, one has to impose a separate condition at the triple junctions where three grain boundaries meet [20]. Note, that at the equilibrium state, the energy is minimized, which implies that a force balance, known as the Herring condition, holds at the triple junctions. Therefore, Herring condition is the natural boundary condition for the network at the equilibrium state. However, during the evolution of the grain boundary network, the normal velocity of the interface is proportional to a driving force. Thus, unlike the equilibrium state, there is no natural boundary condition for an evolutionary system, and one has to be defined. A conventional choice is the Herring condition [8, 9, 20, 19], and reference therein. There are several analytical studies about grain boundary motion by mean curvature with the Herring condition at the triple junctions, see for instance [20, 23, 25, 26]. There is computational work too, [32, 33, 5, 14, 13, 12, 2].

A basic assumption in the theory and simulations of the grain growth is the motion of the grain boundaries themselves and not the motion of the triple junctions. However, recent experimental work indicates that the motion of triple junctions together with anisotropy of the grain boundary network can have an important effect on the grain growth [6], and see also a recent research on dynamics of line defects [34, 35, 31]. The current work is a continuation of our previous work...
where we proposed the model for the evolution of planar grain boundaries with dynamic lattice misorientations and with the triple junction drag. The goal here is to analyze the large time asymptotic behavior of the model proposed in [15].

The paper is organized as follows. In Sections 2-4, we discuss important details and properties of the model for the grain boundary motion. In Sections 5-6, we show the global existence and large time asymptotic behavior of the considered model under assumption of a single triple junction. In Section 7, we discuss the extension of the theory to the grain boundary network with multiple junctions. Finally, in Section 8, we present several numerical experiments to illustrate the obtained theoretical results.

2. Review of the Model

In this article we consider the large time asymptotic behavior of the model for the evolution of the planar grain boundary network with the dynamic lattice misorientations and the triple junctions drag. Thus, here, we first review the model which was originally proposed in [15].

Let us first assume a case of a single triple junction and study the large time asymptotic behavior of the following system, where we relaxed curvature effect by assuming that the mobility of each grain boundary $\mu_j \to \infty$ (see [15]):

\[
\begin{align*}
\frac{d\alpha_j}{dt} &= -(|b^{(j+1)}(t)| + |b^{(j)}(t)|)\alpha_j^{(j)} + |b^{(j+1)}(t)|\alpha_j^{(j+1)} + |b^{(j)}(t)|\alpha_j^{(j-1)}, \\
\frac{da}{dt} &= \sum_{j=1}^{3} \left( 1 + \frac{1}{2} \left( \alpha_{j-1}^{(j)}(t) - \alpha_j^{(j)}(t) \right)^2 \right) \frac{b^{(j)}}{|b^{(j)}|}, \\
a(t) + b^{(j)}(t) &= x^{(j)},
\end{align*}
\]  

In the above system (2.1), $\alpha_j^{(j)} = \alpha_j^{(j)}(t) : [0, \infty) \to \mathbb{R}$, $a = a(t) : [0, \infty) \to \mathbb{R}^2$ are time-dependent functions of the orientations of the grains and a position of the triple junction, respectively, and $x^{(j)}$ are positions of the end points of the grain boundaries, see Fig. 1. We consider $b^{(j)}$ as a grain boundary (which coincides in this model with a tangent vector to the curve/boundary, not necessarily a unit vector), and study the effects of misorientations and the triple junctions on the mobility of the grain boundaries, see Figure 1. Further, we assume that, $\alpha_0^{(0)} = \alpha_3^{(3)}$, $\alpha_4^{(4)} = \alpha_1^{(1)}$ and $b_4^{(4)} = b_1^{(1)}$, for simplicity. We also use below notation $|\cdot|$ for a standard euclidean vector norm. Note that, the system of equations (2.1) is derived from the energetic variational principle for the grain boundary energy which is defined as,

\[
E = \sum_{j=1}^{3} \left( 1 + \frac{1}{2} \left( \alpha_{j-1}^{(j)} - \alpha_j^{(j)} \right)^2 \right) |b^{(j)}|.
\]  

We later review the derivation of the system (2.1) in Section 3.

To explain the idea of the main result of this work, consider the equilibrium state of the grain boundary energy (2.2), namely,

\[
\frac{\delta E}{\delta \alpha_j^{(j)}} = 0, \quad \frac{\delta E}{\delta a} = 0.
\]  

(2.3)
Assume, for each $i = 1, 2, 3$,

\begin{equation}
\left| \sum_{j=1, j\neq i}^{3} \frac{x^{(j)} - x^{(i)}}{|x^{(j)} - x^{(i)}|} \right| > 1.
\end{equation}

The assumption (2.4) includes, that there is no line such that all fixed points $x^{(j)}, j = 1, 2, 3$ are on the single line. Furthermore, (2.4) is equivalent to the condition that the triangle with vertices $x^{(1)}x^{(2)}x^{(3)}$, all three angles are less than $\frac{2\pi}{3}$. Next, from the assumption (2.4), associated equilibrium system (2.3) becomes,

\begin{equation}
\begin{cases}
\sum_{j=1}^{3} \frac{b^{(j)}}{|b^{(j)}|} = 0, \\
\alpha^{(j)} + b^{(j)} = x^{(j)}, \quad j = 1, 2, 3.
\end{cases}
\end{equation}

Our main result is the exponential stability for the equilibrium state (2.5). That is, if the initial misorientations are sufficiently small and the initial triple junction is sufficiently close to the equilibrium state position of the triple junction, then, the solution of (2.1) exists globally in time and it exponentially converges to the equilibrium state solution of (2.5). Our strategy of the proof is to show a priori estimate for the position of the triple junction, and then study of the linearized problem (2.1) around the equilibrium state. With the aid of the assumption (2.4), the equilibrium state system (2.5) is uniquely solvable. Moreover, the equilibrium state is also the energy minimizing state. Thus, we can obtain a priori estimate for the position of the triple junction and a full convergence result for large time asymptotics of the solution. Again thanks to (2.4), the linearized operator of (2.1) is degenerate if and only if there are no misorientation effects, that is, all $\alpha^{(j)}$ are the same. Thus, we can obtain the exponential stability for the equilibrium state.
Figure 2. The figure illustrates the model of the equilibrium state (2.5). There are no misorientation effects on the grain boundaries. A solution of (2.5) is unique under the assumption (2.4), and it minimizes the total length of $\Gamma_\infty^{(j)}$.

We also consider large time asymptotic behavior of grain boundary networks. In general, the uniqueness for the equilibrium state is not known and there might be critical events (disappearance of the grains, grain boundaries, etc. [3, 4, 5, 2]). We study the large time asymptotics for the grain boundary network around the energy minimizing state. We explain global existence and large time asymptotic behavior for the grain boundary network in Section 7.

3. Brief Discussion on the Derivation of the System of Grain Boundary Motion

In this section, we briefly review main details of the derivation of the system of the grain boundary motion (2.1). The complete details can be found in earlier work [15, Section 2]. To understand the effects of the misorientations and the triple junction on the evolution of the grain boundaries, we start by considering three grain boundaries $\Gamma_t^{(1)}$, $\Gamma_t^{(2)}$, and $\Gamma_t^{(3)}$ as curves,

\[(3.1) \quad \Gamma_t^{(j)} : \xi^{(j)}(s,t), \quad 0 \leq s \leq 1, \quad t > 0, \quad j = 1, 2, 3,\]

satisfying boundary conditions imposed at the triple junction $a(t)$ (where these three grain boundaries meet),

\[(3.2) \quad a(t) := \xi^{(1)}(0,t) = \xi^{(2)}(0,t) = \xi^{(3)}(0,t), \quad \text{and} \quad \xi^{(j)}(1,t) = x^{(j)}, \quad j = 1, 2, 3,\]

for fixed $x^{(j)} \in \mathbb{R}^2$. Denote, a tangent vector $b^{(j)} = \xi^{(j)}_s$ and a normal vector $n^{(j)} = Rb^{(j)}$ (not necessarily the unit vectors) to each curve, where $R$ is the rotation matrix through $\pi/2$. Note that, the parameter $s$ is not the arc length parameter of $\Gamma_t^{(j)}$. For simplicity, we assume that the grain boundary energy density is independent of the normal direction/vector of $\Gamma_t^{(j)}$. Thus, let $\sigma = \sigma(\alpha) \geq 0$ be a given nonnegative grain boundary/interfacial energy density function, and we define the total grain boundary energy for the system, see Fig. [3] as,

\[(3.3) \quad E(t) = \sum_{j=1}^{3} \int_0^1 \sigma(\Delta^{(j)}(s))|b^{(j)}(s)| \, ds = \sum_{j=1}^{3} \int_{\Gamma_t^{(j)}} \sigma(\Delta^{(j)}(s)) \, d\mathcal{H}^1.\]
Here, we denote a misorientation angle, $\Delta(j) \alpha = \alpha^{(j-1)} - \alpha^{(j)}$, and we assume, $\alpha^{(0)} = \alpha^{(3)}$. The measure $H^1$ is the 1-dimensional Hausdorff measure, which is the same as the length element of the grain boundaries when the grain boundaries are sufficiently smooth. To simplify the notations, we later denote $\sigma(j) := \sigma(\Delta(j) \alpha)$.

Let us define grain boundary motion to ensure dissipation of the total grain boundary energy (3.3). Let $\hat{\cdot}$ be the normalization operator of vectors, e.g. $\hat{n}^{(j)} = \frac{n^{(j)}}{|n^{(j)}|}$. Then, in [15, Section 2], it was shown that the rate of change of the grain boundary energy at time $t$ due to grain boundary motion is given as,

$$
\frac{d}{dt} E(t) = \sum_{j=1}^{3} \left( \int_{0}^{1} \sigma^{(j)} \hat{b}^{(j)} \cdot \frac{d}{ds} \frac{d \xi^{(j)}}{dt} - ds + \int_{0}^{1} \sigma^{(j)} \frac{d(\Delta \alpha^{(j)})}{dt} |b^{(j)}| ds \right)
$$

$$
= - \sum_{j=1}^{3} \int_{0}^{1} \left( \sigma^{(j)} \hat{b}^{(j)} \right) s \cdot \frac{d \xi^{(j)}}{dt} ds + \sum_{j=1}^{3} \int_{0}^{1} \sigma^{(j)} \frac{d(\Delta \alpha^{(j)})}{dt} |b^{(j)}| ds
$$

$$
- \sum_{j=1}^{3} \sigma^{(j)} \hat{b}^{(j)}(0,t) \cdot \frac{d a}{dt}(t).
$$

(3.4)

Since $\sigma^{(j)}$ is independent of $s$, we have

$$
\left( \sigma^{(j)} \hat{b}^{(j)} \right) s = \sigma^{(j)} \kappa^{(j)} |b^{(j)}| \hat{n}^{(j)},
$$

where $\kappa^{(j)}$ is the curvature of $\Gamma^{(j)}_t$.

Now to ensure that the entire system (3.4) is dissipative, namely $\frac{d}{dt} E(t) \leq 0$, we impose the Mullins equation (or curvature-driven growth) for the evolution of each curve:

$$
\nu_n^{(j)} = \mu \sigma^{(j)} \kappa^{(j)} \text{ on } \Gamma^{(j)}_t, \quad j = 1, 2, 3,
$$

(3.5)
where \( v_n^{(j)} \) is the normal velocity of the curve/grain boundary \( \Gamma_t^{(j)} \), and \( \mu > 0 \) is a positive constant.

Additionally, we enforce the evolution equation for the grain’s orientation \( \alpha^{(j)}(t) \),

\[
\frac{d\alpha^{(j)}}{dt} = -\gamma \left( \int_0^1 \left( |\sigma_\alpha^{(j+1)}| |\mathbf{b}^{(j+1)}| - |\sigma_\alpha^{(j)}| |\mathbf{b}^{(j)}| \right) ds \right), \quad j = 1, 2, 3,
\]

where \( \gamma > 0 \) is a positive constant.

Finally, we impose the following dynamic boundary condition at the triple junction \( \mathbf{a}(t) \),

\[
\frac{d\mathbf{a}}{dt}(t) = \eta \sum_{j=1}^3 \sigma^{(j)} \dot{\mathbf{b}}^{(j)}(0, t), \quad t > 0,
\]

where \( \eta > 0 \) is a constant.

**Remark 3.1.** Note, that if we consider the relaxation limit \( \eta \to \infty \), then we obtain

\[
0 = \sum_{j=1}^3 \sigma^{(j)} \dot{\mathbf{b}}^{(j)}(0, t), \quad t > 0,
\]

which is called the Herring condition (or force balance condition). The Herring condition \(3.8\) is a natural boundary condition when we consider the equilibrium state for the grain boundary system. On the other hand, for the evolution of the grain boundaries, to have a well-posed system, we have to impose some condition for the triple junction, see for example [20, 15].

From the Mullins equation \(3.5\), the evolution of the orientations \(3.6\) and the dynamic boundary condition at the triple junction \(3.7\), we obtain the energy dissipation principle for the considered grain boundary system,

\[
\frac{d}{dt} E(t) = -\sum_{j=1}^3 \int_{\Gamma_t^{(j)}} \frac{1}{\mu} v_n^{(j)} \, d\mathcal{H}^1 - \frac{1}{\eta} \left( \frac{d\mathbf{a}}{dt}(t) \right)^2 - \frac{1}{\gamma} \sum_{j=1}^3 \left( \frac{d\alpha^{(j)}}{dt} \right)^2 \leq 0.
\]

Next, combining equations \(3.5\), \(3.6\), and \(3.7\), we obtain the following system of geometric evolution equations to model grain boundary motion,

\[
\left\{ \begin{array}{l}
\v_n^{(j)} = \mu \sigma^{(j)} \kappa^{(j)}, \quad \text{on } \Gamma_t^{(j)}, \quad t > 0, \quad j = 1, 2, 3, \\
\frac{d\alpha^{(j)}}{dt} = -\gamma \left( \int_0^1 \left( \sigma_\alpha^{(j+1)}|\mathbf{b}^{(j+1)}| - \sigma_\alpha^{(j)}|\mathbf{b}^{(j)}| \right) ds \right), \quad j = 1, 2, 3, \\
\frac{d\mathbf{a}}{dt}(t) = \eta \sum_{j=1}^3 \sigma^{(j)} \dot{\mathbf{b}}^{(j)}(0, t), \quad t > 0,
\end{array} \right.
\]

\[
\Gamma_t^{(j)} : \xi^{(j)}(s, t), \quad 0 \leq s \leq 1, \quad t > 0, \quad j = 1, 2, 3,
\]

\[
a(t) = \xi^{(1)}(0, t) = \xi^{(2)}(0, t) = \xi^{(3)}(0, t), \quad \text{and} \quad \xi^{(j)}(1, t) = \mathbf{x}^{(j)}, \quad j = 1, 2, 3.
\]

Next, to study the effect of the dynamics of the misorientations and triple junction point, we relax a curvature effect on the evolution of grain boundary, namely, we take a relaxation limit as \( \mu \to \infty \). Hence, the grain boundaries become the line segments,

\[
\left\{ \begin{array}{l}
\xi^{(j)}(s, t) = a(t) + s \mathbf{b}^{(j)}(t), \quad 0 \leq s \leq 1, \quad t > 0, \quad j = 1, 2, 3, \\
a(t) + \mathbf{b}^{(j)}(t) = \mathbf{x}^{(j)}, \quad j = 1, 2, 3.
\end{array} \right.
\]
Further, for simplicity, we also assume,
\begin{equation}
(3.11) \quad \sigma(\Delta^{(j)} \alpha) = 1 + \frac{1}{2}(\Delta^{(j)} \alpha)^2 = 1 + \frac{1}{2}(\alpha^{(j-1)} - \alpha^{(j)})^2.
\end{equation}

However, we anticipate that results obtained in this work will hold true for the surface energy given by the convex function. Then, \( \alpha^{(j)} = \Delta \alpha^{(j)} = \alpha^{(j-1)} - \alpha^{(j)} \) hence we deduce
\begin{equation}
(3.12) \quad \frac{d \alpha^{(j)}}{dt} = -\gamma (|b^{(j+1)}(t)| + |b^{(j)}(t)|) \alpha^{(j)} + |b^{(j+1)}(t)| \alpha^{(j-1)} + |b^{(j)}(t)| \alpha^{(j-1)}, \quad j = 1, 2, 3.
\end{equation}

We also set \( \gamma = \eta = 1 \) for simplicity. Then, from (3.10), we obtain the system of equations (2.1). The associated grain boundary energy for the system (2.1) is,
\begin{equation}
(3.13) \quad E(t) = \sum_{j=1}^{3} \left( 1 + \frac{1}{2} (\alpha^{(j-1)} - \alpha^{(j)})^2 \right) |b^{(j)}(t)|.
\end{equation}

The model (2.1) is derived by taking the relaxation limit \( \mu \to \infty \) of the problem (3.10). The study of the original problem (3.10) will be a part of the future work. We emphasize that the model (2.1) has highly nonlinear structure: the nonlinearity of the problem (2.1) comes from the dynamics of the triple junctions of the grain boundaries.

4. Preliminaries

In this section, for the reader’s convenience, we review some known results, as well as established additional properties for the system, defined in (2.1). In particular, we review local existence and a priori estimates results for the model (2.1), more details can be found in [15].

Let \( x^{(j)} \in \mathbb{R}^2 \), \( \alpha_0 \in \mathbb{R}^3 \), and \( a_0 \in \mathbb{R}^2 \) be given initial data and we consider the initial value problem of (2.1), namely
\begin{equation}
(4.1) \quad \begin{cases}
\frac{d \alpha}{dt} = -\mathbb{B}(t) \alpha, \quad t > 0, \quad \alpha(t) = t \left( \alpha^{(1)}(t), \alpha^{(2)}(t), \alpha^{(3)}(t) \right), \\
\mathbb{B}(t) = \begin{pmatrix}
|b^{(1)}(t)| + |b^{(2)}(t)| & -|b^{(2)}(t)| & -|b^{(1)}(t)| \\
-|b^{(2)}(t)| & |b^{(2)}(t)| + |b^{(3)}(t)| & -|b^{(3)}(t)| \\
-|b^{(1)}(t)| & -|b^{(3)}(t)| & |b^{(3)}(t)} + |b^{(1)}(t)|
\end{pmatrix}, \\
\frac{d a}{dt} = \sum_{j=1}^{3} \left( 1 + \frac{1}{2} (\alpha^{(j-1)} - \alpha^{(j)})^2 \right) \frac{b^{(j)}}{|b^{(j)}|}, \quad t > 0, \\
a(t) + b^{(j)}(t) = x^{(j)}, \quad t > 0, \quad j = 1, 2, 3, \\
\alpha(0) = \alpha_0, \quad a(0) = a_0.
\end{cases}
\end{equation}

To study the properties of the coefficient matrix of the equation of \( \alpha \) in (4.1), we consider a matrix for \( c_1, c_2, c_3 \in \mathbb{R} \)
\begin{equation}
(4.2) \quad \mathbb{C} := \begin{pmatrix}
c_1 + c_2 & -c_2 & -c_1 \\
-c_2 & c_2 + c_3 & -c_3 \\
-c_1 & -c_3 & c_3 + c_1
\end{pmatrix}.
\end{equation}

Lemma 4.1 ([15], Lemma 3.1). The eigenvalues of the matrix \( \mathbb{C} \) defined by (4.2) are
\[ 0 \text{ and } c_1 + c_2 + c_3 \pm \sqrt{\frac{1}{2}((c_1 - c_2)^2 + (c_2 - c_3)^2 + (c_3 - c_1)^2)}. \]
If $c_1, c_2, c_3 \geq 0$, then the matrix $C$ is non-negative definite. Furthermore, if $c_1, c_2, c_3 > 0$, then the zero eigenvalue of $C$ is simple, and $\lambda(1, 1, 1)$ is an eigenvector associated with the zero eigenvalue.

From Lemma 4.1, one can also obtain,

Corollary 4.2 ([15 Lemma 3.2]). For $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3$,

$$|C\alpha| \leq 3(|c_1| + |c_2| + |c_3|)|\alpha|.$$  

(4.3)

Now, we are ready to state local existence and uniqueness result.

Proposition 4.3 (Local existence [15 Theorem 4.1]). Let $x^{(1)}, x^{(2)}, x^{(3)} \in \mathbb{R}^2$, $a_0 \in \mathbb{R}^2$, and $\alpha_0 \in \mathbb{R}^3$ be initial data. Assume (2.4) for $i = 1, 2, 3$, and let $a_\infty$ be a solution of (2.5). Further, assume that for all $j = 1, 2, 3$,

$$\|a_0 - a_\infty\| < \frac{1}{2} |b^{(j)}_\infty|.$$  

(4.4)

Then, there exists a unique local solution $(\alpha, a)$ of (2.1) on $0 \leq t < T$. Moreover, we have that,

$$\|\alpha\|_{C([0, T])} \leq 2|\alpha_0|, \quad \|a - a_\infty\|_{C([0, T])} \leq 2|a - a_\infty|,$$

(4.5)

$$T \geq \min \left\{ \frac{1}{12 \sum_{j=1}^{3} |b^{(j)}_\infty|}, \frac{|a_0 - a_\infty|}{3(1 + 8|\alpha_0|^2)}, \frac{1}{56|\alpha_0|^2}, \frac{1}{8 \sum_{j=1}^{3} \frac{1}{|b^{(j)}_\infty| - 2|a_0 - a_\infty|}} \right\}.$$

To show Proposition 4.3, the contraction mapping principle is employed [15]. Note that, the assumption (4.4) guarantees that the equation for the triple junction $a$ in (2.1) is consistent in a classical sense for a short time interval. In other words, the point vector $a$ does not coincide with the Dirichlet point $x^{(j)}$, and stays as the triple junction. Note also, if one can obtain a priori bounds for $|\alpha|$ and $|a - a_\infty|$ from (4.5), then the solution given by Proposition 4.3 can be extended globally in time.

Next we review some a priori estimates for (2.1). Since our problem (2.1) ensures the energy dissipation principle (3.9), one can obtain,

Proposition 4.4 (Energy dissipation [15 Proposition 5.1]). Let $(\alpha, a)$ be a solution of (2.1) on $0 \leq t \leq T$, and let $E$, given by (2.13), be the grain boundary energy of the system. Then, for all $0 < t \leq T$,

$$E(t) + \int_{0}^{t} \left| \frac{d\alpha}{dt}(\tau) \right|^2 d\tau + \int_{0}^{t} \left| \frac{da}{dt}(\tau) \right|^2 d\tau = E(0).$$  

(4.6)

The estimate (4.6) is obtained by taking the derivative of the energy $E(t)$ and using the system (2.1).

We also have a maximum principle for the orientation $\alpha^{(j)}$.

Proposition 4.5 (Maximum principle [15 Proposition 5.2]). Let $(\alpha, a)$ be a solution of (2.1) on $0 \leq t \leq T$. Then, for all $0 < t \leq T$,

$$|\alpha(t)|^2 + 2 \int_{0}^{t} (\mathcal{B}(\tau) \alpha(\tau) \cdot \alpha(\tau)) d\tau = |\alpha_0|^2.$$  

(4.7)

In particular, the maximum principle $|\alpha(t)| \leq |\alpha_0|$ holds.
The estimate (4.7) can be obtained by multiplying the equation of $\alpha$ in (2.1) by $\alpha$ and integrating in time. Since, matrix $B$ is nonnegative definite for all $t > 0$, the maximum principle for the orientations $\alpha$ holds.

Lastly, we show that the sum of the orientations is also preserved.

**Lemma 4.6** (Preserving total orientations). Let $(\alpha, a)$ be a solution of (2.1) on $0 \leq t \leq T$. Then, for all $0 < t \leq T$,

$$\alpha^{(1)}(t) + \alpha^{(2)}(t) + \alpha^{(3)}(t) = \alpha^{(1)}_0 + \alpha^{(2)}_0 + \alpha^{(3)}_0. \quad (4.8)$$

**Proof.** Since, matrix $B$ is symmetric and $B(1, 1, 1) = 0$, we obtain that,

$$\frac{d}{dt}(\alpha^{(1)} + \alpha^{(2)} + \alpha^{(3)}) = (\alpha_t \cdot (1, 1, 1)) = -B\alpha \cdot (1, 1, 1) = -\alpha \cdot (1, 1, 1). \quad \Box$$

Above, we discussed some known results about the system (4.1), [15]. In the current work, we employ these results to show the existence of the global solution, and obtain the large time asymptotic behavior of (4.1).

5. Global existence

In this section, existence theory for a global in time solution of (2.1) is presented. As mentioned earlier, to show the global existence we need to derive a priori estimates for $|\alpha|$ and $|a - a_\infty|$. We already have a priori estimates for $|\alpha|$, see Proposition 4.5 (the maximum principle). Therefore, the main objective here is to obtain a priori estimates for $|a - a_\infty|$.

Define,

$$C_1 := \inf \left\{ \sum_{j=1}^{3} |a - x^{(j)}| : |a - a_\infty| \geq \frac{1}{2} |b^{(j)}_\infty|, \; j = 1, 2, 3 \right\}. \quad (5.1)$$

Since $a_\infty$ is the unique minimizer of

$$f(a) = \sum_{j=1}^{3} |a - x^{(j)}|, \quad a \in \mathbb{R}^2 \quad \text{and} \quad f : \mathbb{R}^2 \to \mathbb{R} \text{ is continuous, we have,}$$

$$0 < \sum_{j=1}^{3} |b^{(j)}_\infty| = f(a_\infty) < C_1. \quad (5.2)$$

Next lemma gives some a priori estimate for the triple junction $a$.

**Lemma 5.1** (Boundedness of the triple junction). Assume that an initial data $(\alpha_0, a_0)$ satisfies,

$$E(0) = \sum_{j=1}^{3} \left( 1 + \frac{1}{2} (\alpha_0^{(j-1)} - \alpha_0^{(j)})^2 \right) |a_0 - x^{(j)}| < C_1. \quad (5.4)$$

Let $(\alpha, a)$ be a solution of (2.1) on $0 \leq t \leq T$. Then, we have that,

$$|a(t) - a_\infty| < \frac{1}{2} |b^{(j)}_\infty| = \frac{1}{2} |a_\infty - x^{(j)}| \quad (5.5)$$

for $j = 1, 2, 3$, and for any $0 \leq t \leq T$. 

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Proof. Assume, there is \( 0 \leq t_1 \leq T \), such that, \( |a(t_1) - a_\infty| \geq \frac{1}{2} |b_\infty^{(j)}|, \ j = 1, 2, 3 \). Then (5.1) and Proposition 4.4 (energy dissipation) lead,
\[
C_1 \leq \sum_{j=1}^{3} |a(t_1) - x^{(j)}| = \sum_{j=1}^{3} |b^{(j)}(t_1)| \leq \sum_{j=1}^{3} \left( 1 + \frac{1}{2} (\alpha^{(j-1)}_0 - \alpha^{(j)}_0)^2 \right) |a_0 - x^{(j)}|,
\]
which contradicts (5.4). \( \square \)

**Remark 5.2.** Note, if we assume (5.4), then we have,
\[
\sum_{j=1}^{3} |a_0 - x^{(j)}| \leq \sum_{j=1}^{3} \left( 1 + \frac{1}{2} (\alpha^{(j-1)}_0 - \alpha^{(j)}_0)^2 \right) |a_0 - x^{(j)}| < C_1,
\]
thus, \( |a_0 - a_\infty| < |b_\infty^{(j)}|/2 \). Hence, the assumption (4.4) will be automatically deduced.

**Remark 5.3.** Assumption (5.4) is a kind of smallness for the initial data \((\alpha_0, a_0)\). If the initial misorientations are sufficiently small and the initial triple junction point is sufficiently close to the equilibrium triple junction point, then we obtain (5.4).

Now we are in position to establish the global existence of the solution of (2.1).

**Theorem 5.4** (Global existence). Let \( x^{(1)}, x^{(2)}, x^{(3)} \in \mathbb{R}^2, a_0 \in \mathbb{R}^2, \) and \( a_0 \in \mathbb{R}^3 \) be the initial data for the system (2.1). Assume (2.4), and let \( a_\infty \) be a unique solution of the equilibrium system (2.5). Further, assume condition (5.4). Then there exists a unique global in time solution \((\alpha, a)\) of (2.1).

**Proof.** We need to show that the solution given by Proposition 4.3 extends globally in time. Let \((\alpha, a)\) be a solution of (2.1) on \( 0 \leq t \leq T \). By Lemma 5.1, we obtain \( |a(T) - a_\infty| < \frac{1}{2} |b_\infty^{(j)}| \).

Due to proposition 4.4 (energy dissipation), we also have,
\[
E(T) = \sum_{j=1}^{3} \left( 1 + \frac{1}{2} (\alpha^{(j-1)}(T) - \alpha^{(j)}(T))^2 \right) |a(T) - x^{(j)}| \leq E(0) < C_1.
\]

In addition, from Proposition 4.5 (maximum principle), we have that \( |\alpha(T)| \leq |\alpha_0| \), hence we can extend the solution globally in time. \( \square \)

In the above proof, a key argument is how to obtain the a priori estimate for the triple junction \( a \). An energy smallness condition (5.4) plays an important role to obtain the a priori estimate for the solution of (2.1).

### 6. Large time asymptotic behavior

We study large time behavior of the global solution given by the Theorem 5.4. We first show large time asymptotics of the solution of (2.1).

**Proposition 6.1.** Let \( x^{(1)}, x^{(2)}, x^{(3)} \in \mathbb{R}^2, a_0 \in \mathbb{R}^2, \) and \( a_0 \in \mathbb{R}^3 \) be the initial data for the system (2.1). Suppose the same assumptions as in Theorem 5.4. Define \( a_\infty \) as,
\[
\alpha_\infty := \frac{\alpha^{(1)}_0 + \alpha^{(2)}_0 + \alpha^{(3)}_0}{3}.
\]

Let \( a_\infty \) be a solution of the equilibrium system (2.5) and \((\alpha, a)\) be a time global solution of (2.1). Then,
\[
\alpha(t) \to \alpha_\infty (1, 1, 1), \quad a(t) \to a_\infty,
\]
(6.2)
as \( t \rightarrow \infty \).

**Proof.** Consider arbitrary time sequence \( t_k \rightarrow \infty \). From the Proposition 4.5 (maximum principle), Lemma 5.1 (boundedness of the triple junction), and the Proposition 4.4 (energy dissipation), we have a convergent subsequence (denoted by the same \( t_k \rightarrow \infty \)) such that,

\[
\alpha(t_k) \rightarrow \alpha_{\infty, *}, \quad a(t_k) \rightarrow a_{\infty,*},
\]

\[
\frac{da}{dt} \rightarrow 0, \quad \frac{da}{dt} \rightarrow 0,
\]

and,

\[
|a_{\infty, *} - a_\infty| \leq \frac{1}{2} |a_{\infty} - x^{(j)}|,
\]

for some \( \alpha_{\infty,*} \in \mathbb{R}^3 \) and \( a_{\infty,*} \in \mathbb{R}^2 \). We have to show \( \alpha_{\infty,*} = \alpha_\infty \) and \( a_{\infty,*} = a_\infty \). Taking the same limit with respect to \( t_k \) in the equation (2.1), from (6.3) we obtain,

\[
\begin{align*}
0 &= -B_{\infty,*} \alpha_{\infty,*}, \quad \alpha_{\infty,*} = \{ \alpha_{\infty,*}^{(1)}, \alpha_{\infty,*}^{(2)}, \alpha_{\infty,*}^{(3)} \}, \\
B_{\infty,*} &= \begin{pmatrix}
|b_{\infty,*}^{(1)}| + |b_{\infty,*}^{(2)}| & -|b_{\infty,*}^{(2)}| & -|b_{\infty,*}^{(1)}| \\
-|b_{\infty,*}^{(2)}| & |b_{\infty,*}^{(2)}| + |b_{\infty,*}^{(3)}| & -|b_{\infty,*}^{(3)}| \\
-|b_{\infty,*}^{(1)}| & -|b_{\infty,*}^{(3)}| & |b_{\infty,*}^{(3)}| + |b_{\infty,*}^{(1)}|
\end{pmatrix}, \\
0 &= \sum_{j=1}^{3} \left( 1 + \frac{1}{2} (\alpha_{\infty,*}^{(j-1)} - \alpha_{\infty,*}^{(j)})^2 \right) \frac{b_{\infty,*}^{(j)}}{|b_{\infty,*}^{(j)}|} b_{\infty,*}^{(j)}, \\
a_{\infty,*} = x^{(1)} - b_{\infty,*}^{(1)} = x^{(2)} - b_{\infty,*}^{(2)} = x^{(3)} - b_{\infty,*}^{(3)}.
\end{align*}
\]

The kernel of \( B_{\infty,*} \) is spanned by \(^t (1, 1, 1)\). Indeed, by (6.4), we have that,

\[
|b_{\infty,*}^{(j)}| = |x^{(j)}| \geq |x^{(j)} - a_\infty| - |a_\infty - a_{\infty,*}| \geq \frac{1}{2} |x^{(j)} - a_\infty| > 0.
\]

Thus, due to Lemma 4.1, the kernel of \( B_{\infty,*} \) is spanned by \(^t (1, 1, 1)\). From Lemma 4.1 (6.5), and (6.1) we find, \( \alpha_{\infty,*} = \alpha_\infty \)\(^t (1, 1, 1)\). Again using (6.5), we obtain that,

\[
0 = \sum_{j=1}^{3} \frac{b_{\infty,*}^{(j)}}{|b_{\infty,*}^{(j)}|}.
\]

Therefore, by uniqueness of the Fermat-Torricelli problem, we obtain that, \( a_{\infty,*} = a_\infty \) (cf. the Fermat-Forricelli Problem [7, Theorem 18.28])).

\[\square\]

**Lemma 6.2** (Linearized problem). The linearized problem of (2.1) around \((\alpha_\infty, a_\infty)\) is given as,
\[ \frac{d\alpha_L}{dt} = -\mathbb{B}_\infty \alpha_L, \quad \mathbb{B}_\infty = \begin{pmatrix} |b^{(1)}_\infty| + |b^{(2)}_\infty| & -|b^{(2)}_\infty| & -|b^{(1)}_\infty| \\ -|b^{(2)}_\infty| & |b^{(2)}_\infty| + |b^{(3)}_\infty| & -|b^{(3)}_\infty| \\ -|b^{(3)}_\infty| & -|b^{(3)}_\infty| & |b^{(3)}_\infty| + |b^{(1)}_\infty| \end{pmatrix}. \]

(6.6)

\[
\begin{aligned}
\frac{d\alpha_L}{dt} &= -\sum_{j=1}^{3} \left( \frac{1}{|b^{(j)}_\infty|} \left( I - \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|} \otimes \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|} \right) \right) a_L =: -L_a a_L, \\
\sum_{j=1}^{3} \delta^{(j)}_\infty &= 0.
\end{aligned}
\]

**Proof.** To obtain the linearized problem (6.6), we consider,

\[
\alpha(t) = \alpha_\infty + \varepsilon \alpha_L(t), \quad a(t) = a_\infty + \varepsilon a_L(t),
\]

in (2.1), and take a derivative with respect to \( \varepsilon \). It is easy to show the equation for \( \alpha_L \) (the first equation in (6.6)) and the equation for \( \delta^{(j)}_\infty \) (the third equation in (6.6)). We will elaborate on some details of the right-hand side of the equation for \( a_L \) (the second equation in (6.6)). Hence, we compute,

\[
\begin{aligned}
\frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \left( \sum_{j=1}^{3} \left( 1 + \frac{\varepsilon^2}{2} \left( \alpha_L^{(j-1)}(t) - \alpha_L^{(j)}(t) \right)^2 \right) \frac{b^{(j)}}{|b^{(j)}|} \right) &= \frac{d}{d\varepsilon} \bigg|_{\varepsilon=0} \left( \sum_{j=1}^{3} \left( 1 + \frac{\varepsilon^2}{2} \left( \alpha_L^{(j-1)}(t) - \alpha_L^{(j)}(t) \right)^2 \right) \frac{x^{(j)} - a_\infty - \varepsilon a_L}{x^{(j)} - a_\infty - \varepsilon a_L} \right) \\
&= \left( \sum_{j=1}^{3} \varepsilon \left( \alpha_L^{(j-1)}(t) - \alpha_L^{(j)}(t) \right)^2 \frac{x^{(j)} - a_\infty - \varepsilon a_L}{x^{(j)} - a_\infty - \varepsilon a_L} \right) \\
&\quad + \left( 1 + \frac{\varepsilon^2}{2} \left( \alpha_L^{(j-1)}(t) - \alpha_L^{(j)}(t) \right)^2 \right) \left( \frac{-a_L}{x^{(j)} - a_\infty - \varepsilon a_L} + \frac{(x^{(j)} - a_\infty - \varepsilon a_L) \cdot a_L}{(x^{(j)} - a_\infty - \varepsilon a_L)^3} (x^{(j)} - a_\infty - \varepsilon a_L) \right) \bigg|_{\varepsilon=0} \\
&= \sum_{j=1}^{3} \left( \frac{-a_L}{|b^{(j)}_\infty|} + \frac{b^{(j)}_\infty \cdot a_L}{|b^{(j)}_\infty|^3} a^{(j)}_\infty \right) = -\sum_{j=1}^{3} \frac{1}{|b^{(j)}_\infty|} \left( a_L - \frac{b^{(j)}_\infty \cdot a_L}{|b^{(j)}_\infty|^2} b^{(j)}_\infty \right).
\end{aligned}
\]

Note, that the term,

\[
\frac{b^{(j)}_\infty \cdot a_L}{|b^{(j)}_\infty|^2} = \left( \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|^2} \right) \cdot a_L = \left( \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|} \otimes \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|} \right) a_L,
\]

where \( \otimes \) denotes the outer product of two vectors. \( \square \)

**Proposition 6.3.** Let \( \alpha_L \) be a solution of (6.6). Assume that, \( \alpha_L(0) \cdot (1, 1, 1) = 0 \). Then, there exists a positive constant \( C_2 > 0 \) such that,

\[
|\alpha_L(t)| \leq e^{C_2 t} |\alpha_L(0)|.
\]

**Proof.** Using (6.6) we have that,

\[
\frac{d}{dt} (\alpha_L \cdot (1, 1, 1)) = -\mathbb{B}_\infty \alpha_L \cdot (1, 1, 1) = -\alpha_L \cdot \mathbb{B}_\infty (1, 1, 1) = 0,
\]
hence, $\alpha_L \cdot (1, 1, 1) = \alpha_L(0) \cdot (1, 1, 1) = 0$. Define,

$$
(6.9) \quad C_2 := |b_{10}^{(1)}| + |b_{10}^{(2)}| + |b_{10}^{(3)}| - \sqrt{\frac{1}{2} \left( (|b_{10}^{(1)}| - |b_{10}^{(2)}|)^2 + (|b_{10}^{(2)}| - |b_{10}^{(3)}|)^2 + (|b_{10}^{(3)}| - |b_{10}^{(1)}|)^2 \right)},
$$

which is the smallest positive eigenvalue of $B_{10}$ due to Lemma 4.1. Since $|b^{(j)}| > 0$ and $\alpha_L \cdot (1, 1, 1) = 0$, from Lemma 4.1 we find that $\alpha_L$ is spanned by the eigenvectors associated with the positive eigenvalues of $B_{10}$. Thus, we obtain,

$$
\frac{d}{dt}|\alpha_L(t)|^2 = -2B_{10} \alpha_L(t) \cdot \alpha_L(t) \leq -2C_2|\alpha_L(t)|^2.
$$

By the Gronwall’s inequality, we obtain (6.8). □

**Lemma 6.4.** There exists a positive constant $C_3 > 0$ such that,

$$
(6.10) \quad L_a := \sum_{j=1}^{3} \frac{1}{|b_{10}^{(j)}|} \left( I - \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \otimes \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \right) \geq C_3 I.
$$

**Proof.** For $\xi \in \mathbb{R}^2$, we have that,

$$
\left( \sum_{j=1}^{3} \frac{1}{|b_{10}^{(j)}|} \left( I - \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \otimes \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \right) \xi \cdot \xi \right) = \sum_{j=1}^{3} \frac{1}{|b_{10}^{(j)}|} \left( |\xi|^2 - \left( \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \cdot \xi \right)^2 \right) \geq 0,
$$

hence, we obtain (6.10) with some $C_3 \geq 0$.

Assume now that $C_3 = 0$, then there is $\xi_0 \in \mathbb{S}^1$ such that,

$$
\sum_{j=1}^{3} \frac{1}{|b_{10}^{(j)}|} \left( 1 - \left( \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \cdot \xi_0 \right)^2 \right) = 0.
$$

Thus, $\xi_0$ is parallel to all $b_{10}^{(j)}$ for $j = 1, 2, 3$. This is contradiction to the dimension of $\mathbb{R}^2$. □

The convergence rate of the global solution to the equilibrium state depends on the decay rate of the linearized solution, hence it is important to give estimates for the constant $C_3$. We will give an explicit form of $C_3$ in Appendix A.

Similar to the result of Proposition 6.3, we obtain,

**Proposition 6.5.** Let $a_L(t)$ be a solution of (6.6). Then,

$$
(6.11) \quad |a_L(t)| \leq e^{-C_3 t} |a_L(0)|,
$$

for all $t > 0$, and the constant $C_3 > 0$ is given by Lemma 6.4.

Denote $C_4 := \min\{C_2, C_3\}$. Define $\alpha$ and $a_p$ as,

$$
(6.12) \quad \alpha = \alpha_\infty + \alpha_p, \quad a = a_\infty + a_p.
$$

Then $\alpha_p$ and $a_p$ satisfy,

$$
(6.13) \quad \begin{cases}
(\alpha_p)_t = -B_\alpha = -B_\infty \alpha_p - (B - B_\infty) \alpha_p, \\
(a_p)_t = -L_a a_p + \sum_{j=1}^{3} \left( \frac{1}{|b_{10}^{(j)}|} \left( I - \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \otimes \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \right) a_p + \left( 1 + \frac{1}{2} (\alpha^{(j-1)} - \alpha^{(j)})^2 \right) \frac{b_{10}^{(j)}}{|b_{10}^{(j)}|} \right),
\end{cases}
$$

where $L_a$ is defined as in (6.10).
Lemma 6.6. Let $\alpha_p$ and $a_p$ be defined by (6.12). Then for all $t > 0$

\begin{equation}
  e^{C_4 t} |a_p(t)| \leq |a_p(0)| + 9 \int_0^t e^{C_4 s} |a_p(s)||a_p(s)| \, ds.
\end{equation}

**Proof.** By the Duhamel principle for (6.13), we have,

\begin{equation}
  a_p(t) = e^{-tB_{\infty}} a_p(0) + \int_0^t e^{-(t-s)B_{\infty}} (B(s) - B_{\infty}) a_p(s) \, ds.
\end{equation}

Since $\alpha_0 \cdot (1, 1, 1) = \alpha_{\infty} \cdot (1, 1, 1)$ and $(1, 1, 1) \in \text{Ker}(\mathcal{B}(s) - \mathcal{B}_{\infty})$ for all $s > 0$, $a_p(0)$ and $(\mathcal{B}(s) - \mathcal{B}_{\infty}) a_p(s)$ are perpendicular to the vector $(1, 1, 1)$ for all $s > 0$. By Proposition 6.3 we also obtain that,

\begin{equation}
  |e^{-tB_{\infty}} a_p(0)| \leq e^{-C_4 t} |a_p(0)|, \quad |e^{-(t-s)B_{\infty}} (\mathcal{B}(s) - \mathcal{B}_{\infty}) a_p(s)| \leq e^{-C_4(t-s)} |(\mathcal{B}(s) - \mathcal{B}_{\infty}) a_p(s)|.
\end{equation}

By Corollary 6.2 we have,

\begin{equation}
  |(\mathcal{B}(s) - \mathcal{B}_{\infty}) a_p(s)| \leq 3 \left( |b^{(1)}(s) - b^{(1)}_{\infty}| + |b^{(2)}(s) - b^{(2)}_{\infty}| + |b^{(3)}(s) - b^{(3)}_{\infty}| \right) |a_p(s)| \leq 9 |a_p(s)| |a_p(s)|
\end{equation}

Using the estimates (6.16) and (6.17) in (6.15), we obtain the result (6.14). \hfill \Box

Lemma 6.7. Let $\alpha_p$ and $a_p$ be defined as in (6.12). Then, there are positive constants $C_5 > 0$ and $\varepsilon_1 > 0$, such that, if $|a_p(t)| < \varepsilon_1$ for all $t > 0$, then,

\begin{equation}
  e^{C_4 t} |a_p(t)| \leq |a_p(0)| + \int_0^t e^{C_4 s} \left( 2 |a_p|^2 + C_5 |a_p|^2 \right) \, ds,
\end{equation}

for all $t > 0$.

**Proof.** By Duhamel principle for (6.13), we have,

\begin{equation}
  a_p(t) = e^{-t\alpha} a_p(0) + \int_0^t e^{-(t-s)\alpha} F(s) \, ds,
\end{equation}

where

\begin{equation}
  F(s) := \sum_{j=1}^3 \left( \frac{1}{|b^{(j)}_{\infty}|} \left( I - \frac{b^{(j)}_{\infty}}{|b^{(j)}_{\infty}|} \otimes \frac{b^{(j)}_{\infty}}{|b^{(j)}_{\infty}|} \right) a_p + \left( 1 + \frac{1}{2} (\alpha^{(j-1)} - \alpha^{(j)})^2 \right) \frac{b^{(j)}_{\infty}}{|b^{(j)}_{\infty}|} \right).
\end{equation}

By Lemma 6.4 and Proposition 6.5 we obtain,

\begin{equation}
  |a_p(t)| \leq e^{-C_4 t} |a_p(0)| + \int_0^t e^{-C_4(t-s)} |F(s)| \, ds.
\end{equation}

Next, note that,

\[
  \frac{1}{|b^{(j)}|} = \frac{1}{|x^{(j)} - a|} = \frac{1}{|x^{(j)} - a_{\infty} - a_p|} = \frac{1}{|b^{(j)}_{\infty} - x a_p|}_{x=1}.
\]

Hence, by the Taylor expansion of $1/|b^{(j)}|$ around $b^{(j)}_{\infty}$, we obtain,

\[
  \frac{1}{|b^{(j)}|} = \frac{1}{|x^{(j)} - a|} = \frac{1}{|b^{(j)}_{\infty}|} + \frac{1}{|b^{(j)}_{\infty}|^2} \hat{b}^{(j)}_{\infty} \cdot a_p + O(|a_p|^2), \quad \text{as } |a_p| \to 0.
\]
Thus, we have that,

\[ \frac{b^{(j)}}{|b^{(j)}|} = \left( \frac{1}{|b^{(j)}_\infty|} + \frac{1}{|b^{(j)}_\infty|^2} \hat{r}^{(j)} \cdot a_p + O(|a_p|^2) \right) (b^{(j)}_\infty - a_p) \]

(6.22)

\[ = \hat{r}^{(j)}_\infty + \frac{1}{|b^{(j)}_\infty|} \left( (\hat{r}^{(j)}_\infty \cdot a_p) \hat{r}^{(j)}_\infty - a_p \right) + O(|a_p|^2) \]

\[ = \hat{r}^{(j)}_\infty + \frac{1}{|b^{(j)}_\infty|} \left( \hat{r}^{(j)}_\infty \otimes \hat{r}^{(j)}_\infty - I \right) a_p + O(|a_p|^2), \quad \text{as } |a_p| \to 0. \]

Using, (6.22) and (6.6) in (6.20), we obtain,

\[ F(s) = \frac{1}{2} \sum_{j=1}^{3} (\alpha^{(j-1)} - \alpha^{(j)}) \hat{r}^{(j)} + O(|a_p|^2) \]

(6.23)

\[ = \frac{1}{2} \sum_{j=1}^{3} (\alpha^{(j-1)}_p - \alpha^{(j)}_p) \hat{r}^{(j)} + O(|a_p|^2), \quad \text{as } |a_p| \to 0. \]

Hence, there are \( C_5 > 0 \) and \( \varepsilon_1 > 0 \) such that, if \( |a_p| < \varepsilon \),

\[ |F(s)| \leq \frac{1}{2} \sum_{j=1}^{3} (\alpha^{(j-1)}_p - \alpha^{(j)}_p)^2 + C_5 |a_p|^2 \]

(6.24)

\[ \leq \sum_{j=1}^{3} \left( (\alpha^{(j-1)}_p)^2 + (\alpha^{(j)}_p)^2 \right) + C_5 |a_p|^2 = 2 |\alpha_p|^2 + C_5 |a_p|^2. \]

Using estimate (6.24) in (6.21), we conclude with the desired estimate on \( a_p(t) \). \( \square \)

**Theorem 6.8.** There is a small constant \( \varepsilon_2 > 0 \) such that, if \( |\alpha_p(0)| + |a_p(0)| < \varepsilon_2 \), then the associated global solution \((\alpha, a)\) of the system (2.1) satisfies,

\[ |\alpha(t) - \alpha_\infty| + |a(t) - a_\infty| \leq C_6 e^{-C_6 t}, \]

(6.25)

for some positive constant \( C_6 > 0 \).

**Proof.** We define \( V(t) := e^{C_i t}|\alpha_p(t)| \) and \( W(t) := e^{C_i t}|a_p(t)| \). Next, fix \( 0 < \varepsilon_2 < \varepsilon_1/2 \), where the constant \( \varepsilon_1 \) is given in Lemma 6.7, and assume that \( |\alpha_p(0)| + |a_p(0)| < \varepsilon_2 \). Now, assume \( V(t) + W(t) < 2\varepsilon_2 \) for \( 0 \leq t < t_0 \) and \( V(t_0) + W(t_0) = 2\varepsilon_2 \). Note that, \( W(t) < \varepsilon_1 \) for \( 0 < t < t_0 \), thus we can apply Lemma 6.7. Therefore, from (6.14), (6.18) and that \( V(t), W(t) \leq 2\varepsilon_2 \) for \( 0 < t \leq t_0 \), we obtain,

\[ V(t) + W(t) \leq V(0) + W(0) + \frac{C_2}{2} \int_0^t e^{-C_4 s} (V^2(s) + W^2(s)) \, ds \]

(6.26)

\[ \leq \varepsilon_2 + C_7 \varepsilon_2 \int_0^t e^{-C_4 s} (V(s) + W(s)) \, ds, \]

where \( C_7 = 2C_5 + 13 > 0 \). Applying the Gronwall’s inequality to (6.26), we have that,

\[ V(t) + W(t) \leq \varepsilon_2 + C_7 \varepsilon_2^2 \int_0^t e^{-C_4 s} \exp \left( C_7 \varepsilon_2 \int_s^t e^{-C_4 u} \, du \right) \, ds, \quad 0 \leq t \leq t_0. \]

(6.27)
Hence, we can easily obtain that,

\[ C_7 \varepsilon_2^2 \int_0^t e^{-C_4 s} \exp \left( C_7 \varepsilon_2 \int_s^t e^{-C_4 u} du \right) \, ds \leq \frac{C_7 \varepsilon_2^2}{C_4} \exp \left( \frac{C_7 \varepsilon_2}{C_4} \right). \]

Thus, if we take \( \varepsilon_2 > 0 \) sufficiently small as,

\[ (6.28) \quad \frac{C_7 \varepsilon_2}{C_4} \exp \left( \frac{C_7 \varepsilon_2}{C_4} \right) < 1, \]

then we deduce that \( V(t_0) + W(t_0) < 2\varepsilon_2 \), which contradicts the definition of \( t_0 \) above. Therefore, \( V(t) + W(t) \) is bounded for \( 0 < t < \infty \), and we obtain (6.25). \( \Box \)

**Remark 6.9.** Note that our argument is based on the uniqueness of the equilibrium state for the system (2.5). Otherwise, we can not recover full convergence in time as in the Proposition 6.1. However, thanks to the uniqueness of the equilibrium state (2.5), we can consider the linearized problem (6.6) around the equilibrium state, and we can obtain the exponential uniform estimate (6.25) for the solution of the system (2.1).

**Remark 6.10.** If we do not assume \( \eta = \gamma = 1 \) (see Sect. 3, (3.10)-(3.13)), the order of the decay for \( C_4 \) should be proportional to \( \gamma \) and \( \eta \). In fact, \( C_4 \) is given by \( \min \{ \gamma C_2, \eta C_3 \} \), where \( C_2, C_3 \) is defined by (6.9) and (6.10), respectively.

Note also, that by Theorem 6.8, we obtain exponential decay of the total grain boundary energy to the equilibrium energy, that is

**Corollary 6.11.** Under the same assumption as in Theorem 6.8, the associated grain boundary energy \( E(t) \) satisfies,

\[ (6.29) \quad E(t) - E_\infty \leq C_8 e^{-C_4 t}, \]

for some positive constant \( C_8 > 0 \).

**Proof.** Since \( \alpha_\infty^{(1)} = \alpha_\infty^{(2)} = \alpha_\infty^{(3)} \), we obtain

\[ (6.30) \quad E(t) - E_\infty = \sum_{j=1}^3 \left( (1 + \frac{1}{2} (\alpha^{(j-1)}(t) - \alpha^{(j)}(t))^2) |b^{(j)}(t)| - |b_\infty^{(j)}| \right) \leq \sum_{j=1}^3 \left( |b^{(j)}(t) - b_\infty^{(j)}| + (\alpha^{(j-1)}(t) - \alpha_\infty^{(j-1)})^2 + (\alpha^{(j)}(t) - \alpha_\infty^{(j)})^2 |b^{(j)}(t)| \right). \]

Using the dissipation estimate (6.25), we obtain (6.29). \( \Box \)

**Remark 6.12.** 1. Note that, based on the estimate (6.30), the dominate part of the energy decay seems to be due to the the triple junction effect, \( |b^{(j)}(t) - b_\infty^{(j)}| \). In fact, in the numerical experiments, it was observed that the energy dissipation due to misorientation effect is much smaller than the energy dissipation due to the triple junctions effect.

2. Note also, that the obtained exponential decay to equilibrium, see estimates (6.25) and (6.29) is obtained by considering linearized problem, Lemma 6.2. Consideration of the nonlinear problem instead could lead to power laws estimates for the decay rates. See also discussion and numerical experiments in Sec. 8.
7. Extension to Grain Boundary Network

In this section, we extend our results to a grain boundary network \( \{ \Gamma_t^{(j)} \} \). As before, the lattice orientation of the single grain is denoted as \( \{ \alpha^{(k)} \} \) and triple junctions are defined as \( \{ a^{(l)} \} \). We identify the lattice orientation \( \alpha^{(k)} \) with the grain itself. As in, for example, [15], we define the total grain boundary energy of the network, like,

\[
E(t) = \sum_j \int_{\Gamma_t^{(j)}} \sigma(\Delta^{(j)} \alpha) \, d\mathcal{H}^1,
\]

where \( \Delta^{(j)} \alpha \) is a misorientation, a difference between the lattice orientation of the two neighboring grains which form the grain boundary \( \Gamma^{(j)} \). Then, similar to the argument in Section 3, we have that,

\[
\frac{d}{dt} E(t) = -\sum_j \int_{\Gamma_t^{(j)}} \frac{d}{ds} T^{(j)} \, d\mathcal{H}^1 \sum_k \frac{\partial E}{\partial \alpha^{(k)}} \frac{d\alpha^{(k)}}{dt} - \sum_l \sum_{a^{(l)} \in \Gamma_t^{(j)}} T^{(j)} \cdot \frac{d a^{(l)}}{d t},
\]

where

\[
T^{(j)} = \sigma(\Delta^{(j)} \alpha) \hat{b}^{(j)}.
\]

Note that, on the triple junction \( a^{(l)} \), the direction of the unit tangent vector \( \hat{b}^{(j)} \) is given from the triple junction itself towards the grain boundary \( \Gamma_t^{(j)} \).

We impose the local evolutions law for the network using equations (3.5)-(3.7). Hence, we obtain the system for the evolution of the grain boundary network as follows,

\[
\begin{align*}
\forall j, j \neq k \in \{ \Gamma_t^{(j)} \} \\
\frac{d\alpha^{(k)}}{dt} &= -\gamma \frac{\delta E}{\delta \alpha^{(k)}} , \\
\frac{d a^{(l)}}{dt} &= \eta \sum_{a^{(l)} \in \Gamma_t^{(j)}} \left( \sigma^{(j)} \frac{b^{(j)}}{|b^{(j)}|} \right),
\end{align*}
\]

One can show (see [15]), that the energy dissipation estimate for the network of the grain boundaries is given as,

\[
\frac{d}{dt} E(t) = -\frac{1}{\mu} \sum_j \int_{\Gamma_t^{(j)}} |v_n^{(j)}|^2 \, d\mathcal{H}^1 - \frac{1}{\gamma} \sum_k |d\alpha^{(k)}|^2 - \frac{1}{\eta} \sum_l |d a^{(l)}|^2.
\]

As in [15], we consider the relaxation parameters, \( \mu \to \infty, \gamma = \eta = 1 \), and the interfacial energy density,

\[
\sigma(\alpha) = 1 + \frac{1}{2} \alpha^2.
\]
Then, the problem (7.4) becomes,

\[
\begin{aligned}
\Gamma_t^{(j)} & \text{ is a line segment between some } a_t^{(l,j,1)} \text{ and } a_t^{(l,j,2)}, \\
\frac{d\alpha^{(k)}}{dt} &= - \sum_{\text{grain with } \alpha^{(k')}} \frac{\left| \Gamma_t^{(j)} \right| (\alpha^{(k)} - \alpha^{(k')})}{\Gamma_t^{(j)} \text{ is formed by the two grains with } \alpha^{(k)} \text{ and } \alpha^{(k')}} \\
\frac{da^{(l)}}{dt} &= \sum_{a^{(l)} \in \Gamma_t^{(j)}} \left( \sigma^{(j)} \frac{b^{(j)}}{|b^{(j)}|} \right).
\end{aligned}
\] 

\tag{7.7}

To obtain the global solution of the system (7.7), we first assume that there are no critical events in the system (for example, disappearance of the grains and/or grain boundaries during coarsening of the system), and we consider an associated energy minimizing state, \((\alpha_\infty^{(k)}, a_\infty^{(l)})\) of (7.7). Then, \((\alpha_\infty^{(k)}, a_\infty^{(l)})\) satisfies,

\[
\begin{aligned}
\Gamma_\infty^{(j)} & \text{ is a line segment between some } a_\infty^{(l,j,1)} \text{ and } a_\infty^{(l,j,2)}, \\
0 &= - \sum_{\text{grain with } \alpha^{(k')}} \frac{\left| \Gamma_\infty^{(j)} \right| (\alpha_\infty^{(k)} - \alpha_\infty^{(k')})}{\Gamma_\infty^{(j)} \text{ is formed by the two grains with } \alpha^{(k)} \text{ and } \alpha^{(k')}} \\
0 &= \sum_{a_\infty^{(l,j)} \in \Gamma_\infty^{(j)}} \left( \sigma_\infty^{(j)} \frac{b_\infty^{(j)}}{|b_\infty^{(j)}|} \right).
\end{aligned}
\] 

\tag{7.8}

Hence, the total energy \(E_\infty\) of the grain boundary network (7.8) is

\[
E_\infty = \sum_j \left( 1 + \frac{1}{2} \left( \Delta^{(j)} a_\infty \right)^2 \right) |b_\infty^{(j)}| = \inf \left\{ \sum_j \left( 1 + \frac{1}{2} \left( \Delta^{(j)} a \right)^2 \right) |b^{(j)}| \right\}.
\] 

\tag{7.9}

Remark 7.1. Note, we assume in (7.7)-(7.8) that the total number of grains, grain boundaries and triple junctions is the same as in the initial configuration (assumption of no critical events in the network).

If there is a neighborhood \(U^{(l)} \subset \mathbb{R}^2\) of \(a_\infty^{(l)}\) such that

\[
E_\infty < \sum_j |b^{(j)}|
\] 

\tag{7.10}

for all \(a^{(l)} \in U^{(l)}\), one can obtain a priori estimate for the triple junctions, and, hence, obtain the time global solution of (7.7). Note that, the assumption (7.10) is related to the boundary condition of the line segments \(\Gamma_t^{(j)}\). Further, if the energy minimizing state is unique, then we can proceed with the same argument as in Lemma 5.1 and obtain the global solution (7.7) near the energy minimizing state.

Example 7.2. Note that, the solution of (7.8) may not be unique even though grain orientation is constant (misorientation is zero). The total grain boundary energy in the left plot is different from the one in the right plot, see Figure 4.

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The asymptotics of the grain boundary networks are rather nontrivial. Our arguments rely on the uniqueness of the equilibrium state (2.5), but we do not know the uniqueness of solutions of the equilibrium state for the grain boundary network (7.10). Thus, in general we cannot take a full limit of the large time asymptotic behavior. Concluding the above arguments, we have

**Theorem 7.3.** In a grain boundary network (7.7), assume that the initial configuration is sufficiently close to an associated energy minimizing state (7.8), (7.9), and (7.10). Then, there is a global solution \((\alpha^{(k)}, a^{(l)})\) of (7.7). Furthermore, there exists a time sequence \(t_n \to \infty\) such that \((\alpha^{(k)}(t_n), a^{(l)}(t_n))\) converges to an associated equilibrium configuration (7.8).

**8. Numerical Experiments**

Here, we present several numerical experiments to illustrate the effect of the dynamic misorientation and the effect of the mobility of the triple junctions as discussed in Secs. 6, 7. In particular, we show the consistency between theoretical and numerical decay rates of the total grain boundary energy, and of the triple junctions and misorientations to their steady-states, see Sec. 6, (6.25), (6.29), Remark 6.12, Sec. 7 and Fig. 6, Fig. 8, Fig. 10 and Fig. 12. However, note that based on the results of the numerical experiments, Fig. 6, Fig. 8, Fig. 10, the numerical decay rates for the total grain boundary energy look more like power law, \(t^{-1}\), and the decay rate similar to the power law of \(t^{-0.5}\) for the results in Fig. 12 rather than the exponential decay as seen from the theory. Note also, that the numerically observed decay rates increase with the mobility of the triple junctions, and the decay rates are also consistent with the growth of the average area under finite mobility of the triple junctions, see Fig. 7, Fig. 9, Fig. 11 (left plots), and with the growth of the average area under Herring condition/infinite mobility, see Fig. 13 (left plot), respectively. The difference between the numerical experiments and the presented theory could be due to finite curvature effect in numerical experiments, the effect of the critical events on the dissipation rates, as well as due to theoretical consideration of the linearized problem, see Sec. 6. Moreover, we study the impact of the dynamic misorientation and the mobility of the triple junctions on the Grain Boundary Character Distribution Statistics (GBCD), see Fig. 7, Fig. 9, Fig. 11 and Fig. 13 (right plots). The GBCD (in our context) is an
empirical statistical measure of the relative length (in 2D) of the grain boundary interface with a given lattice misorientation. It is a leading candidate to characterize texture of the boundary network. The reader can consult, for example, [3, 4, 5, 2, 6] for more details about GBCD and the theory of GBCD.

Figure 5. Time instance from the simulation of the 2D grain boundary network with dynamic/time-dependent orientation (zoom view).

Figure 6. Three runs of 2D trial with 10000 initial grains: (a) Left plot, Total grain boundary energy plots from 3 runs (solid black) versus fitted exponential decaying function $y(t) = 414.3 \exp(-11.11t)$ (dashed blue) and power law decaying function $y(t) = -209.6 + 77.96(0.1242 + t)^{-1}$ (magenta); (b) Right plot, Triple Junctions and Orientations plots from 3 runs (solid black) (see formula (6.25)) versus exponential decaying function $y(t) = 55 \exp(-7t)$ (dashed black). Plots illustrate consistency between theoretical results and results of the numerical model. Mobility of the triple junctions is $\eta = 5$. 
Figure 7. Three runs of 2D trial with 10000 initial grains: (a) Left plot, Growth of the average area of the grains from 3 runs (solid black) versus fitted quadratic polynomial function $y(t) = 0.1727t^2 + 0.001914t + 0.0003766$ (dashed magenta); (b) Right plot, steady-state GBCD averaged over 3 runs (blue curve) versus Boltzmann distribution with “temperature” $\sigma \approx 0.0489$ (red curve). The growth of the average area is consistent with the energy decay, Fig. 6, left plot. Mobility of triple junctions is $\eta = 5$.

For the numerical experiments in this work, we consider simulation of 2D grain boundary network with the dynamic orientations and with the dynamic boundary conditions at the triple junctions, see Fig. 5 and Sec. 7 (7.4). Note, that in numerical experiments, see Figs. 6-11, all three independent relaxation time scales in (7.4), $\mu$, $\gamma$ and $\eta$ (length, misorientation and position of the triple junction) are kept finite, and in the numerical experiment, see Figs. 12-13, we let $\eta \rightarrow \infty$, by considering Herring condition at the triple junctions. The scale $\gamma$ is set to 1 in all numerical experiments below. The considered numerical experiments are based on the extension of the numerical algorithm developed in [5, 2]. For more details about computational model based on Mullins equations (curvature driven growth), the reader can consult, for example [5, 2] (note, that in [5, 2], $\gamma \rightarrow \infty$ and $\eta \rightarrow \infty$). In the numerical tests, we assume that the network reaches statistical steady-state when approximately 80% of grains disappeared from the system.

In our numerical experiments, the results are consistent with the theory in Secs. 6-7 (note that, for the evolution of the misorientations and triple junctions, in numerical tests, we track only grains and triple junctions that “survive” through the entire time of the simulation). Furthermore, from all numerical experiments with dynamic misorientation and with different triple junction mobilities, we observe that the steady-state GBCD is well-approximated by the Boltzmann Distribution for the grain boundary energy density, similar to the work in [3, 4, 5, 2, 6], but more careful analysis need to be done to understand the relation between GBCD and different relaxation time scales.
Figure 8. Three runs of 2D trial with 10000 initial grains: (a) Left plot, Total grain boundary energy plots from 3 runs (solid black) versus fitted exponential decaying function $y(t) = 413.8 \exp(-21.69t)$ (dashed blue) and power law decaying function $y_1(t) = -194.5 + 37.5367(0.06132 + t)^{-1}$ (magenta); (b) Right plot, Triple Junctions and Orientations plots from 3 runs (solid black) (see formula (6.25)) versus exponential decaying function $y(t) = 55 \exp(-10t)$ (dashed black). Plots illustrate consistency between theoretical results and results of the numerical model. Mobility of the triple junctions is $\eta = 10$.

Remark 8.1. Note, that the proposed model of dynamic orientations (7.7) (and, hence, dynamic misorientations), or Langevin type equation if critical events/grain boundaries disappearance events are taken into account) is reminiscent of the recently developed theory for the grain boundary character distribution (GBCD) [3, 4, 5, 2], which suggests that the evolution of the GBCD satisfies a Fokker-Planck Equation. More details will be presented in future studies.

Acknowledgments

The authors are grateful to David Kinderlehrer for the fruitful discussions, inspiration and motivation of the work. Yekaterina Epshteyn and Masashi Mizuno acknowledge partial support of Simons Foundation Grant No. 415673, Yekaterina Epshteyn also acknowledges partial support of NSF DMS-1905463, Masashi Mizuno also acknowledges partial support of JSPS KAKENHI Grant No. 18K13446, Chun Liu acknowledges partial support of NSF DMS-1759535 and NSF DMS-1759536. Yekaterina Epshteyn would like to thank Nihon University for the hospitality during her visit and Masashi Mizuno also would like to thank Penn State University, Illinois Institute of Technology and the University of Utah for the hospitality during his visits.
Figure 9. Three runs of 2D trial with 10000 initial grains: (a) Left plot, Growth of the average area of the grains from 3 runs (solid black) versus fitted quadratic polynomial function \( y(t) = 0.6399t^2 + 0.004625t + 0.000373 \) (dashed magenta); (b) Right plot, steady-state GBCD averaged over 3 runs (blue curve) versus Boltzmann distribution with “temperature” \( \sigma \approx 0.0508 \) (red curve). The growth of the average area is consistent with the energy decay, Fig. 8, left plot. Mobility of triple junctions is \( \eta = 10 \).

Appendix A. Explicit Form of the Decay Rate of the Linearized Problem (6.6)

In this appendix, we give an explicit form of the constant \( C_3 \), which is a minimum eigenvalue of

\[
L_a = \sum_{j=1}^{3} \frac{1}{|b^{(j)}_{\infty}|} \left( I - \frac{b^{(j)}_{\infty}}{|b^{(j)}_{\infty}|} \otimes \frac{b^{(j)}_{\infty}}{|b^{(j)}_{\infty}|} \right).
\]

Since \( L_a \) is 2 dimensional matrix, it is enough to manipulate the trace and the determinant of \( L_a \). The trace of \( L_a \) is easily calculated as

\[
\text{tr } L_a = \sum_{j=1}^{3} \frac{1}{|b^{(j)}_{\infty}|} \left( 2 - \text{tr} \frac{b^{(j)}_{\infty}}{|b^{(j)}_{\infty}|} \otimes \frac{b^{(j)}_{\infty}}{|b^{(j)}_{\infty}|} \right) = \sum_{j=1}^{3} \frac{1}{|b^{(j)}_{\infty}|}.
\]

Next we consider the determinant of \( L_a \). Denote \( b^{(j)}_{\infty} = (b^{(j)}_{\infty,1}, b^{(j)}_{\infty,2}) \), \( b^{(j)}_{\infty} := \frac{b^{(j)}_{\infty,1}}{b^{(j)}_{\infty,2}} \), and \( b^{(j)}_{\infty} = |b^{(j)}_{\infty}| \). Then,

\[
L_a = \sum_{j=1}^{3} \begin{pmatrix}
\frac{1}{b^{(j)}_{\infty}} & -\frac{1}{b^{(j)}_{\infty}} b^{(j)}_{1} b^{(j)}_{2} \\
-\frac{1}{b^{(j)}_{\infty}} b^{(j)}_{1} b^{(j)}_{2} & 1 \end{pmatrix} \begin{pmatrix}
1 - \left( b^{(j)}_{1} \right)^2 \\
1 - \left( b^{(j)}_{2} \right)^2
\end{pmatrix}.
\]
hence,

\[
\det L_{\alpha} = \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} \left( 1 - \left( b_{1}^{(j)} \right)^{2} \right) \right) \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} \left( 1 - \left( b_{2}^{(j)} \right)^{2} \right) \right) - \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} b_{1}^{(j)} b_{2}^{(j)} \right)^{2}
\]

\[
= \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} \left( 1 - \left( b_{1}^{(j)} \right)^{2} \right) \left( 1 - \left( b_{2}^{(j)} \right)^{2} \right) - \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} b_{1}^{(j)} b_{2}^{(j)} \right)^{2}
\]

\[
+ \sum_{j \neq k} \frac{1}{b_{\infty}^{(j)}} b_{\infty}^{(k)} \left( 1 - \left( b_{1}^{(j)} \right)^{2} \right) \left( 1 - \left( b_{2}^{(k)} \right)^{2} \right) - \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} b_{1}^{(j)} b_{2}^{(j)} \right) \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} b_{1}^{(j)} b_{2}^{(j)} \right)
\]

\[
= \sum_{j < k} \frac{1}{b_{\infty}^{(j)}} b_{\infty}^{(k)} \left( 1 - \left( b_{1}^{(j)} \right)^{2} \right) \left( 1 - \left( b_{2}^{(k)} \right)^{2} \right) + \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} b_{1}^{(j)} b_{2}^{(j)} \right)^{2}
\]

\[
+ 1 - \left( b_{1}^{(k)} \right)^{2} - \left( b_{2}^{(j)} \right)^{2} + \left( b_{1}^{(j)} \right)^{2} \left( b_{2}^{(j)} \right)^{2} - 2 \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} b_{1}^{(j)} b_{2}^{(j)} \right) \left( \sum_{j=1}^{3} \frac{1}{b_{\infty}^{(j)}} b_{1}^{(j)} b_{2}^{(j)} \right)
\]

\[
= \sum_{j < k} \frac{1}{b_{\infty}^{(j)}} b_{\infty}^{(k)} \left( b_{1}^{(j)} b_{2}^{(k)} - b_{1}^{(k)} b_{2}^{(j)} \right)^{2}
\]

\[
= \sum_{j < k} \frac{1}{b_{\infty}^{(j)}} b_{\infty}^{(k)} \left( \frac{b_{\infty}^{(j)}}{b_{\infty}^{(j)}} \cdot R_{-\frac{2}{3}} b_{\infty}^{(k)} \right)^{2}.
\]
Figure 11. Three runs of 2D trial with 10000 initial grains: (a) Left plot, Growth of the average area of the grains from 3 runs (solid black) versus fitted quadratic polynomial function \( y(t) = 22.6 t^2 + 0.083 t + 0.00036 \) (dashed magenta); (b) Right plot, steady-state GBCD averaged over 3 runs (blue curve) versus Boltzmann distribution with “temperature” \( \sigma \approx 0.0508 \) (red curve). The growth of the average area is consistent with the energy decay, Fig. 10, left plot.

Mobility of the triple junctions is \( \eta = 100 \).

where \( R_{-\frac{\pi}{2}} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \) is the \(-\frac{\pi}{2}\) rotating matrix, and note that \((b_1^{(j)})^2 + (b_2^{(j)})^2 = 1\). We also know that, \( \left\{ \frac{b^{(k)}_j}{|b^{(k)}_\infty|}, R_{-\frac{\pi}{2}} \frac{b^{(k)}_\infty}{|b^{(k)}_\infty|} \right\} \) is orthonormal basis on \( \mathbb{R}^2 \). Thus for \( 1 \leq j, k \leq 3 \), by Parseval’s identity tells us

\[
\left( \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|}, \frac{b^{(k)}_\infty}{|b^{(k)}_\infty|} \right)^2 + \left( \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|}, R_{-\frac{\pi}{2}} \frac{b^{(k)}_\infty}{|b^{(k)}_\infty|} \right)^2 = 1.
\]

Since,

\[
\frac{b^{(j)}_\infty}{|b^{(j)}_\infty|}, \frac{b^{(k)}_\infty}{|b^{(k)}_\infty|} = -\frac{1}{2} + \frac{3}{2} \delta_{jk},
\]

we finally arrive, for \( j \neq k \)

\[
\left( \frac{b^{(j)}_\infty}{|b^{(j)}_\infty|}, R_{-\frac{\pi}{2}} \frac{b^{(k)}_\infty}{|b^{(k)}_\infty|} \right)^2 = \frac{3}{4}.
\]
Figure 12. Three runs of 2D trial with 10000 initial grains: (a) Left plot, Total grain boundary energy plots from 3 runs (solid black) versus fitted sum of exponential decaying functions $y(t) = 153.9 \exp(-1749t) + 252.6 \exp(-183.9t)$ (dashed blue) and power law decaying function $y_1(t) = -42.75 + 11.27(0.000623 + t)^{-0.5}$ (magenta) compared to exponential decaying function $y_2(t) = 420 \exp(-325t)$ (dashed black); (b) Right plot, Triple Junctions and Orientations plots from 3 runs (solid black) (see formula (6.25)) versus exponential decaying function $y(t) = 55 \exp(-250t)$ (dashed black). Plots illustrate consistency between theoretical results and results of the numerical model. Herring Condition is imposed at the triple junctions $\eta \to \infty$.

Then $C_3 > 0$ in Lemma 6.4 is explicitly given by,

$$C_3 = \frac{1}{2} \left( \text{tr} \ L_a - \sqrt{(\text{tr} \ L_a)^2 - 4(\text{det} \ L_a)} \right)$$

$$= \frac{1}{2} \left( \sum_{j=1}^{3} \frac{1}{|b^{(j)}_\infty|} - \sqrt{\left( \sum_{j=1}^{3} \frac{1}{|b^{(j)}_\infty|} \right)^2 - 3 \left( \sum_{j<k} \frac{1}{|b^{(j)}_\infty|} \frac{1}{|b^{(k)}_\infty|} \right)} \right)$$

$$= \frac{1}{2} \left( \sum_{j=1}^{3} \frac{1}{|b^{(j)}_\infty|} - \sqrt{\frac{1}{2} \sum_{j<k} \left( \frac{1}{|b^{(j)}_\infty|} - \frac{1}{|b^{(k)}_\infty|} \right)^2} \right).$$

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Figure 13. Three runs of 2D trial with 10000 initial grains: (a) Left plot, Growth of the average area of the grains from 3 runs (solid black) versus fitted linear polynomial function \( y(t) = 0.6835t + 0.0003124 \) (dashed magenta); (b) Right plot, steady-state GBCD averaged over 3 runs (blue curve) versus Boltzmann distribution with “temperature” \( \sigma \approx 0.0472 \) (red curve). The growth of the average area is consistent with the energy decay, Fig. 12 left plot. Herring Condition is imposed at the triple junctions \( \eta \to \infty \).

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