Simultaneous Grain Boundary Motion, Grain Rotation, and Sliding in Bicrystalline and Tricrystalline Materials

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Abstract

Grain rotation and grain boundary (GB) sliding are important mechanisms for grain coarsening and plastic deformation in polycrystalline materials with average grain size of few tens of nanometers. We study two-dimensional dynamics of grain rotation and GB sliding coupled with GB migration driven by GB capillary and external stress. The kinetic relations for migration, evolution of grain orientation, relative translational motion of the grains, and junction velocities, all derived within a thermodynamically consistent framework, are developed for several bicrystalline and tricrystalline arrangements. In particular, we consider a bicrystal with two rectangular grains connected by a smooth non-planar GB; and another other one, with a columnar grain embedded inside a larger grain. We also consider a tricrystal composed of a columnar grain embedded at the center of a non-planar GB of a much larger bicrystal made of two rectangular grains. The shape evolution of the embedded grain is examined numerically using a finite difference scheme while emphasizing the role of coupled motion as well as junction mobility and external stress. The shape accommodation at the GB, necessary to maintain coherency, is achieved by allowing for GB diffusion along the boundary.

Keywords: Grain boundary motion; Grain rotation; Grain boundary sliding; Triple junction; Bicrystal; Tricrystal; Nanocrystalline material

1 Introduction

Grain boundaries (GBs) play a central role in various deformation processes involving polycrystalline materials, and more so in influencing the behavior of nanocrystalline (NC) materials with average grain size of few tens of nanometers [21,22,33]. NC materials posses enhanced yield strength, hardness, and diffusivity, but reduced ductility when compared to the coarse-grained polycrystalline materials (average grain size is of the order of microns), mostly due to the presence of a large volume fraction of GBs and triple junctions [22]. Under external stress and interfacial capillarity the microstructure in polycrystals has been observed to evolve thereby altering their overall material properties. The nature
Figure 1: A Schematic to depict the coupling between GB motion and rotation of grain $G_1$ under GB capillary force in a tricrystal. Diagram (a) shows the initial configuration which evolves to (b) at a later time. The outer grains $G_2$ and $G_3$, being much larger than $G_1$, are taken to be stationary (after [32]).

of evolution is however significantly different in coarse grained and NC materials. For instance, grain coarsening is dominated by GB migration in the former but usually accompanied by grain rotation in the latter [17] (see also Chapter 3 of [21] and the references therein). In fact, grain rotation and relative grain translation have been observed to be the dominating plastic deformation mechanisms in NC materials [16][22][33]. Intragranular dislocations, otherwise known to be active carriers of plastic flow in coarse grained materials, have little role in NC materials due to the extremely narrow spacing between the GBs. Local coalescence of grains by rotation can however create space for dislocation movements in NC materials, providing scope for plastic instabilities such as softening and strain localization [11][12][19][20].

Whenever GB migration is coupled with grain rotation and relative grain translation, the resulting motion is called coupled GB motion [5][30][34]. For example, consider an isolated tricrystal arrangement as shown in Figure 1(a) where a grain is embedded at the center of the planar GB of a large bicrystal. In absence of external stress, the embedded grain spontaneously rotates due to GB capilarity, thus changing its orientation, while shrinking to a size shown in Figure 1(b). The embedded grain can disappear either by shrinking to a vanishing volume or by reorienting itself to one of the neighboring grains. The shrinkage rate of the grain is such that the total free energy of the system decreases [5]. Grain rotation can be accomplished through either a pure viscous sliding, or a tangential motion geometrically coupled with GB migration, or a combination of both [5][30]. If the tricrystal is subjected to external stress, the grains can accomplish relative translational motion as well [32]: the center of rotation of the embedded grain then need not remain fixed in space [30]. The presence of triple junctions, which can occupy up to 3% volume fraction in NC materials when the average grain size is around 10 nm (Chapter 5 of [21]), induces drag in the GB dynamics and also affects the coupled motion of GBs [8].

The coupling between grain rotation and GB motion has been extensively studied in two-dimensional (2D) bicrystals where a cylindrical grain is embedded in a larger crystal [5][30][31][34]. The kinetic relations for simultaneous grain rotation and GB motion were proposed by Cahn and Taylor [5] who used them initially to study the evolution of an isolated circular GB and later to non-circular GBs [30]. The coupled motion in such bicrystals was subsequently investigated with molecular dynamics (MD) [31],
phase field (PF) \[34\], and level set \[2\] simulations. Whereas the former two techniques have been used to verify the phenomenon of coupled motion, in addition to providing valuable information regarding the nature of kinetic coefficients, the level set simulations have studied the effect of various kinetic coefficients on the shape evolution of grains. All these studies ignore relative grain translation. More recently, the occurrence of coupled motion has been confirmed in the presence of junctions using MD simulations \[32\]. Under GB capillary force, spontaneous shrinkage and rotation of the embedded grains have been observed. In the presence of external shear stress, a relative translational motion of the grains is also seen to accompany the overall dynamics. It was also shown that the relative rotation can sometimes get locked, thereby preventing coupled motion, but only under suitable geometric conditions (see also \[34\]).

Our aim is to develop a thermodynamically consistent framework to study the coupled GB motion in the presence of triple junctions as driven by GB capillarity and external stress. In doing so we extend earlier works \[2, 5, 30\] which were restricted to bicrystals and therefore neglected junctions. Relative tangential translation at the GBs was also assumed to be absent; as a result the center of rotation of the embedded grains was always fixed. We revisit bicrystalline configurations treated previously with an emphasis on the effect of stress on the coupled GB dynamics through relative translation of grains. Our choice for the 2D tricrystal arrangement, as shown in Figure 1, is motivated by the recent findings in \[32\]. We assume that the grains are rigid, free of defects, and do not possess any stored energy. The defect content as well as the energy density are confined to grain boundaries. Isothermal condition is maintained throughout. The assumption of grain rigidity is justified since we consider the magnitude of the external stress to be much lower than the yield stress. Also, in the present scenario the GBs do not exert any far-field stress and GB capillary exerts very low pressure on the neighbouring grains. The shape accommodation process, required to avoid nucleation of void or interpenetration of the grains at the GBs during relative rotation of the embedded grain, is controlled by allowing for diffusion along the GBs. Bulk diffusion in the grains, as well as across the GBs, is taken to be negligible compared to GB diffusion \[21\]. Furthermore, since both GBs and grains move at much smaller velocities under capillary and small stress than the velocity of sound in that material, the inertial effects are ignored. With these assumptions we derive kinetic relations for GB motion, rotational and translational movements of the grains, and junction dynamics from the respective dissipation inequalities. The driving forces for the coupled motion are obtained from mean curvature, gradient of GB energy, and external stresses. The dynamical equations are all coupled to each other. They are solved numerically to investigate the shape evolution of the shrinking grain for various choices of kinetic parameters, junction mobilities, and stresses. The above assumptions provide the simplest setting to pursue a rigorous study of coupled GB dynamics. The effect of elastic/plastic deformation of the grains and volumetric diffusion should be included in a more realistic model, albeit at the price of increased complexity both in modelling and numerical simulations.

The paper has been organized as follows. After developing the pertinent thermodynamic formalism in Section \[2\] the relevant kinetic relations for two bicrystalline and one tricrystalline configurations are derived in Section \[3\]. These when combined with the constitutive prescription for kinetic coefficients and GB energy, provided in Section \[4\] yields the system of governing equations for the coupled GB dynamics.
The numerical solution is presented in Section 5. Finally, Section 6 concludes our communication.

2 Thermodynamic formalism

The dissipation inequalities at GBs and junctions are now derived within the framework of Gibbs thermodynamics, where various thermodynamic quantities (such as energy, entropy, etc.) defined over interfaces and junctions are understood as excess quantities of the system. We begin by fixing the notation, followed by a formulation of mass and momentum balances, before deriving the consequences of the second law of thermodynamics in terms of various dissipation inequalities.

Consider a 2D control volume $P$ as shown in Figure 2(b) containing three domains $P_1$, $P_2$, and $P_3$, and a junction $J$. $P$ can be thought of as a subdomain in a polycrystalline material, as depicted in Figure 2(a). The boundary separating $P_i$ and $P_{i-1}$ ($i = 1, 2, 3$) has been represented by $\Gamma_i$ ($P_0$ is identified with $P_3$). The normal $n_i$ to $\Gamma_i$ is chosen such that it points into $P_i$. The outer boundary of $P$ and the associated outward normal are denoted by $\partial P$ and $m$, respectively. We parametrize each of the GBs $\Gamma_i$ by an arc-length parameter $s_i$ which initiates at $J$ and increases towards the edge $A_i$. The tangent $t_i$ to $\Gamma_i$ is aligned in the direction of increasing $s_i$. The stress field at the junction is usually singular (cf. [29] and Part H of [14]) and therefore all the analysis is restricted to a punctured domain $P_\epsilon$ which is obtained by removing a small circular region $D_\epsilon$ of radius $\epsilon$ centred at the junction, i.e. $P_\epsilon = P \setminus D_\epsilon$. We denote the periphery of the circular hole in $P_\epsilon$ by $C_\epsilon$ whose outward normal is $m$. The velocity of the curve $C_\epsilon$ approaches the velocity of the junction, denoted by $q$, in the limit $\epsilon \to 0$.

Let $f$ be a field defined in $P$ such that it is continuous everywhere except across $\Gamma_i$. The jump in $f$ across $\Gamma_i$ is denoted by $[f] = f^+ - f^-$, where $f^+$ is the limiting value of $f$ as it approaches $\Gamma_i$ from the side into which $n_i$ points and $f^-$ otherwise. The normal time derivative of a field $g$ defined on $\Gamma_i$ is given by (cf. [6])

$$\dot{g} = \dot{g} + V_i \nabla g \cdot n_i$$

(no summation for the repeated index ‘$i$’ in (1) is considered here and thereafter), where the superposed dot stands for the material time derivative, $V_i$ is the normal velocity of $\Gamma_i$, and $\nabla$ is the gradient operator. It represents the time rate of change of $g$ with respect to an observer sitting on $\Gamma_i$ and moving with the interface in its normal direction.

2.1 Balance of mass

The rate of change of total mass in $P$ in the absence of any external source of mass generation/accretion, with a vanishing mass flux across the boundary $\partial P$, should be balanced by the mass flux through the edges $A_i$, i.e.

$$\frac{d}{dt} \int_P \rho \, da = - \sum_{i=1}^3 (h_i)_{A_i},$$

where $\rho$ is the mass density of the bulk, $h_i$ is the diffusional flux along $\Gamma_i$ in the direction of increasing $s_i$, and $da$ is an infinitesimal area. Using the standard transport and divergence theorems (cf. Equations
Figure 2: (a) Schematic of a polycrystal with a control volume $P$. (b) The control volume $P$ containing three subgrains $P_i$ ($i = 1, 2, 3$), three GBs $\Gamma_i$, and a junction $J$. Normal vectors for the outer boundary of the control volume $\partial P$ and $\Gamma_i$ are denoted by $m$ and $n_i$, respectively. Point $A_i$ denote the edge of $\Gamma_i$ lying on $\partial P$. The broken circle $\mathcal{C}_\epsilon$ is the boundary of the circular disc $\mathcal{D}_\epsilon$ which is removed to obtain the punctured domain $P_\epsilon = P \setminus \mathcal{D}_\epsilon$.

(32.23) and (32.27) in \cite{15}) the following local mass balance relations are imminent:

\begin{align}
\dot{\rho} + \rho \nabla \cdot \mathbf{v} &= 0 \quad \text{in } P_i, \\
\rho \left[ \mathbf{U}_i \right] &= \frac{\partial h_i}{\partial s_i} \quad \text{on } \Gamma_i, \text{ and} \\
\sum_{i=1}^3 h_i &= 0 \quad \text{at } J,
\end{align}

where $\mathbf{v}$ is the particle velocity and $\mathbf{U}_i = \mathbf{V}_i - \mathbf{v} \cdot n_i$ and the relative normal velocity. The term $\nabla \cdot \mathbf{v}$ denotes the divergence of velocity field.

### 2.2 Balance of linear momentum

When GB, grains, and junction inertia is neglected, and the body forces are absent, the balance of linear momentum states that $\int_{\partial P} \mathbf{m} \, dl = 0$, where $\mathbf{m}$ is the symmetric Cauchy stress tensor and $dl$ is the infinitesimal arc length along $\mathcal{C}_\epsilon$. Applying Equation (A5) of \cite{29} this global balance law can be reduced to the following local equations:

\begin{align}
\nabla \cdot \mathbf{m} &= 0 \quad \text{in } P_i, \\
\left[ \mathbf{m} \right] n_i &= 0 \quad \text{on } \Gamma_i, \text{ and} \\
\lim_{\epsilon \to 0} \oint_{\mathcal{C}_\epsilon} \mathbf{m} \, dl &= 0 \quad \text{at } J.
\end{align}

According to \cite{15} the traction is continuous across $\Gamma_i$. On the other hand, \cite{29} implies that even with a singular stress at the junction, the net force on the periphery of $\mathcal{C}_\epsilon$ ($\epsilon \to 0$) is finite. This is known as the standard weak singularity condition which requires $\mathbf{m} \sim \epsilon^{-\zeta}$, where $\zeta \geq 1$ (see Chapter 34 in \cite{14} for further discussion).
2.3 Dissipation inequality

In confirmation with the second law of thermodynamics for isothermal processes, the rate of change of free energy of the control volume $P$ is less than or equal to the total power supplied to $P$:

$$
\sum_{i=1}^{3} \frac{d}{dt} \int_{\Gamma_i} \gamma_i \, dl \leq \int_{\partial P} \mathbf{\sigma} \cdot \mathbf{v} \, dl - \sum_{i=1}^{3} (\mu_i h_i) A_i + \sum_{i=1}^{3} (c_i \cdot w_i) A_i,
$$

(9)

where $\gamma_i$ is the energy density of GB $\Gamma_i$, $\mu$ is the chemical potential of the atoms, and $dl$ is an infinitesimal length along the curve. As noted before, we have ignored bulk free energy as well as volumetric diffusion in the grains. The vector $w_i$ stands for the velocity of edge $A_i$ and $c_i$ is the force conjugate associated with it. The nature of the latter is elaborated below. The first term on R.H.S. of the inequality is the power input into $P$ due to external stress field on its boundary. The second term represents the power input due to additional mass flow. The third term, which is non-standard, represents the power input into $P$ required to ensure that there is no excess entropy generation at the edges $A_i$, thereby restricting the entropy production only at the GBs and the junction. The edges are allowed to carry excess entropy only when they are present on the external surface of the solid, in which case the considered term will not be required. This additional power input will therefore be present only for edges in the interior of the solid. Its form (and hence of $c_i$) will of course depend of the constitutive nature of prescribed excess quantities over GBs and the junction. It can be alternatively interpreted as the power expended by the configurational force $c_i$ at the respective edge. This viewpoint has been adopted in earlier studies (cf. [6,10,29]) within the framework of configuration mechanics.

Our treatment (see also [2,13]) is different from these in that we do not introduce a priori any balance laws associated with configurational forces, nor do we postulate configurational forces as independent fundamental entities alongside the standard Newtonian forces. It should be noted that the final results are identical, irrespective of the chosen standpoint. We will now exploit the above restriction on the nature of entropy production, combined with certain constitutive restrictions on GB energy, to determine $c_i$. This will then be used to obtain local dissipation inequalities at various GBs and the junction.

Applying the transport theorem for the GB (cf. Equation (A8) of [29] and Equation (A5) of [29] in [3]) we obtain

$$
\int_{P} \nabla \cdot (\mathbf{\sigma} \mathbf{v}) \, da + \sum_{i=1}^{3} \int_{\Gamma_i} \left( [\mathbf{\sigma} \mathbf{n}_i \cdot \mathbf{v}] + f_i V_i - \dot{\gamma}_i - \frac{\partial}{\partial s_i} (\mu h_i) \right) \, dl + \sum_{i=1}^{3} (c_i \cdot w_i - \gamma_i W_i) A_i +

\lim_{c \to 0} \int_{\partial \mathcal{C}_i} \mathbf{\sigma} \mathbf{m} \cdot \mathbf{v} \, dl + \sum_{i=1}^{3} (\gamma_i t_i \cdot \mathbf{q} - \mu h_i) J \geq 0,
$$

(10)

where $f_i = \gamma_i \kappa_i$ ($\kappa_i$ is the curvature of $\Gamma_i$), and $W_i$ is the tangential component of the edge velocity $w_i$ at $A_i$. We consider isotropic GB energies such that $\gamma_i = \gamma_i(\theta_i)$, where $\theta_i$ is the misorientation angle at
the boundary $\Gamma_i$. Using (3) – (8) in (10), then yields

$$
\int_P \sigma \cdot \nabla v \, da + \sum_{i=1}^{3} \int_{\Gamma_i} \left( [UE] n \cdot n + \langle \sigma n_i \rangle \cdot [v] \right)_i + f_i V_i - \frac{\partial \gamma_i}{\partial \theta_i} \dot{\theta}_i - h_i \frac{\partial \mu}{\partial s_i} \right) \, dl + \sum_{i=1}^{3} (\gamma_i t_i \cdot q)_J +
$$

$$
\lim_{\epsilon \to 0} \int_{\Gamma_i} \sigma_\epsilon \cdot v \, dl + \sum_{i=1}^{3} (c_i \cdot w_i - \gamma_i W_i)_{A_i} \geq 0, \quad (11)
$$

where $E = -(\rho \mu I + \sigma)$ is the Eshelby tensor in the grains when stored energy is vanishing ($I$ represents the identity tensor), $[v]_i$ is the tangential part of $[v]$, and we have used $\dot{\theta}_i = \dot{\theta}_i$ recalling that the orientation of the various grains remain uniform (since they are defect free). We have also imposed local chemical equilibrium at various boundaries, i.e. $[\mu] = 0$ across $\Gamma_i$ (cf. Section XXXI in [10]).

The three summations in (11) represent the entropy production rate associated with the GBs $\Gamma_i$, the junction $J$, and the edges $A_i$ lying on the boundary of the control volume, respectively. We require the excess entropy production to have no contribution from the edges, hence expecting it to be of the form $\sum_{i=1}^{3} \int_{\Gamma_i} \eta_i \, dl + \eta_J \geq 0$, where $\eta_i$ is the entropy generation rate per unit length of $\Gamma_i$ and $\eta_J$ is the entropy generation rate at the junction. As a consequence, we derive

$$
c_i = \gamma_i t_i, \quad (12)
$$

cf. Equations (17.4) and (17.21) in [10]. The following local dissipation inequalities are then imminent

$$
\sigma \cdot \nabla v \geq 0 \quad \text{in } P_i, \quad (13)
$$

$$
[U E] n \cdot n + \langle \sigma n_i \rangle \cdot [v]_i + f_i V_i - \frac{\partial \gamma_i}{\partial \theta_i} \dot{\theta}_i - h_i \frac{\partial \mu}{\partial s_i} \geq 0 \quad \text{on } \Gamma_i \and (14)
$$

$$
F \cdot q + \lim_{\epsilon \to 0} \int_{\Gamma} \sigma m \cdot v \, dl \geq 0 \quad \text{at } J, \quad (15)
$$

where

$$
F = \sum_{i=1}^{3} \gamma_i t_i \quad (16)
$$

is the driving force for junction motion, cf. [29]. The L.H.S. of these inequalities represent the dissipation rate in the grains (per unit area), at the boundaries (per unit length), and at the junction, respectively. Relation (13) requires the power expenditure in the grains due to stress to be non-negative. When the grains are rigid, as is the case in this paper, the power expenditure in the bulk is identically zero and hence (13) is trivially satisfied. Inequality (14) can be used to distinguish the fluxes (generalized velocities) and the associated driving forces which cause dissipation at a GB. Therefore the average traction drives the relative tangential jump in the velocity between two grains, the mean curvature drives the normal velocity of the GB, and the torque like term $\partial \gamma_i / \partial \theta_i$ drives the evolution of the misorientation. The gradient of the chemical potential acts as a driving force for mass diffusion along the GB. At the junction, according to (15) we see that both adjoining GB energy and the singular stress in its neighbourhood contribute to the net dissipative force.
3 Kinetic relations

Based on the dissipation inequalities (14) and (15) we now derive the kinetic relations for various 2D bicrystal and a tricrystal configurations shown in Figures 3, 4, and 5. The bicrystal shown in Figure 3 (bicrystal-I) is made of two rectangular grains $G_1$ and $G_2$ which are connected by a non-planar GB. Bicrystal-II (Figure 4) is composed of a columnar grain $G_1$ embedded in a larger grain $G_2$. The considered tricrystal (Figure 5) consist of three grains $G_1$, $G_2$, and $G_3$, four boundaries $C_i$, $i = 1, \ldots, 4$, and two junctions $J_1$ and $J_2$.

3.1 Bicrystal-I

As depicted in Figure 3, we parametrize GB $C$ by an arc-length parameter $s$ starting from the edge $E_1$. The position vectors for the edges $E_1$ and $E_2$ are denote by $y_1$ and $y_2$, respectively. We consider a Cartesian coordinate system with basis $\{e_1, e_2, e_3\}$ as shown in the figure. Without loss of generality we assume that the lower grain is stationary, only the upper one is moving with homogeneous velocity $\dot{C}$.

**Pure sliding** We first consider the grains $G_1$ and $G_2$ to undergo GB diffusion accommodated steady-state pure sliding motion along the GB. We also assume the coupling between sliding and normal velocities to be absent. In doing so we recover the results obtained by Raj and Ashby [26] where the upper grain is moving at a velocity $\dot{C} = \dot{C}e_1$. It is assumed that the grains are free of any defects. The natural configuration for the bicrystal will thus be the one where the grains are separated from each other (see [6] for details). Pure sliding will require the normal velocity of the GBs in this natural configuration to vanish, consequently implying the relative normal velocity $U$ to also disappear (cf. Equation 4.5 of [6]). In other words, $V = \dot{C}n_1$, where the normal has been expressed as $n = n_1e_1 + n_2e_2$. As a result, the conjugate force of $U$, i.e. $F = En \cdot n$ must also vanish. Indeed, if we assume $F$ to depend smoothly on $U$ then, under the assumption of decoupled dynamics, we require $\mathcal{D}'(0) = 0$ (superposed prime denotes a derivative), where $\mathcal{D}(U) = U F(U) \geq 0$; this is due to the fact that $\mathcal{D}(U)$
has a minima at $U = 0$. Consequently $F(0) = 0$, i.e.

$$\mu = -\sigma_n / \rho, \quad (17)$$

where $\sigma_n = \sigma \mathbf{n} \cdot \mathbf{n}$. The chemical potential derived in (17) is similar (modulo a constant chemical potential of stress free atoms) to the one introduced earlier by Herring [18].

Under steady-state sliding the thermodynamic state variables do not evolve with time [1]. The entropy production rate given by the left hand side of (14) then must vanish. If the effect of GB curvature is ignored, under steady-state sliding, (14) leads to

$$\langle \sigma \mathbf{n} \rangle \cdot \dot{\mathbf{C}} + \frac{1}{D} \left( \frac{\partial \mu}{\partial s} \right)^2 = 0, \quad (18)$$

where $\dot{\mathbf{C}}_t$ is the tangential part of $\dot{\mathbf{C}}$; we have also used the Fick’s law given by

$$h = -D \frac{\partial \mu}{\partial s}, \quad (19)$$

where $D \geq 0$ is the diffusivity along the GB ‘$\mathcal{C}$’. The equations required to be solved for the sliding rate consist of the mass balance relation, the mechanical equilibrium equations given by (6) and (7), and the condition describing the vanishing dissipation (18) in conjunction with (17).

We now show with an example that our general framework can explain some earlier studies related to GB sliding, which were otherwise motivated by phenomena of creep and superplasticity in crystalline solids. Following Raj and Ashby [26] we consider a sinusoidal GB profile of small amplitude

$$x_2 = A(t) \cos \left( \frac{2\pi x_1}{\lambda} \right), \quad (20)$$

where $A(t)$ is the maximum amplitude and $\lambda$ is the wavelength of the GB. We assume that the amplitude is much smaller than the wavelength, i.e. $A/\lambda << 1$. We adopt the following solution for the normal stress on the GB from [26] (see their Appendix 1)

$$\sigma_n = \frac{\tau \lambda}{\pi A} \sin \left( \frac{2\pi x_1}{\lambda} \right). \quad (21)$$

Using $n_1 = \frac{2\pi A}{\lambda} \sin \left( \frac{2\pi x_1}{\lambda} \right)$, and (17) and (21) in the mass balance relation (22) we obtain

$$\dot{\mathcal{C}} = \frac{2\pi \bar{D}}{A^2},$$

which is in agreement with the result of Raj and Ashby (see Equation (11) in [26]) when the volumetric diffusion is ignored, where $\bar{D} = D / \rho^2$. Using (17) and considering the solutions of the stresses provided in [26] we can easily see that the left hand side of (18) is of the order of $(A/\lambda)^2$, and hence becomes trivial in the present context.
Coupled motion  We next consider a situation where the GB motion in its normal direction is coupled with the sliding of the grains along the GB; cf. [23] for experimental observations and [3] for MD simulations. It is important to note that the chemical potential of the atoms near the GB is no longer given by (17). It can be however computed from the equation of mass balance (4) by integrating it along the GB.

The mass balance given by (4) reduces down to

$$\frac{\partial h}{\partial s} = -\rho \dot{C} \cdot n.$$  (22)

Using $n = e_3 \times t$ and $t = dx/ds$ in (22), we integrate it to obtain

$$h = -\rho \dot{C} \cdot e_3 \times x + k,$$  (23)

where $k$ is an integration constant. Since the bicrystal does not exchange any mass with its surrounding, the diffusion flux must satisfy the boundary conditions $h(y_1) = h(y_2) = 0$. From (23) one can easily check that $h$ will satisfy these boundary conditions if and only if $\dot{C}$ is parallel to $e_1$ (say, $\dot{C} = \dot{C} e_1$) and both the edges $E_1$ and $E_2$ have the same amplitude. Employing this fact in (23) simplifies it to

$$h = -\rho \dot{C} y,$$  (24)

where $y = (x - y_1) \cdot e_2 = (x - y_2) \cdot e_2$. We see that the consideration of the basic statement of the balance of mass given by (22) puts certain restrictions on the geometry of the GB $\mathcal{C}$. However, if one considers that $\mathcal{C}$ has any arbitrary geometry, then a meaningful model perhaps should take volumetric diffusion into account (cf. [26]).

The state of stress is assumed to be uniform throughout the bicrystal and taken to be

$$\sigma = \tau(e_1 \otimes e_2 + e_2 \otimes e_1),$$  (25)

which obviously satisfies the equilibrium equations (6) and (7) and the relevant traction boundary conditions. Equation (8) is irrelevant in the present case as there is no junction in bicrystal-I.

Applying (19) in (24), and then integrating the equation, we get the chemical potential along $\mathcal{C}$ as

$$\mu = -\rho \dot{C} I,$$  (26)

where $I = \int_{s(y_1)}^s y \, dl$. We have taken the chemical potential at the edges as the reference chemical potential, which is zero for there are no normal components of traction on the free surface (assumed to be flat), cf. [18] and Chapter 68 of [15]. The dissipation inequality (14) can presently be rewritten as

$$f V + f_t \dot{C} \geq 0,$$  (27)

where

$$f_t = -\dot{C} I / D n_1 + \tau n_2 + \dot{C} y^2 / D,$$  (28)
and \( n = n_1 e_1 + n_2 e_2 \). From (27), and recalling the Onsager’s reciprocity theorem [25], we postulate the following linear kinetics (motivated from [2, 5])

\[
\dot{C} = \beta V + L f_t, \quad (29)
\]

\[
V = M f + M\beta f_t, \quad (30)
\]

where \( M > 0, L \geq 0, \) and \( \beta \) are GB mobility, translational sliding coefficient, and geometric coupling factor, respectively. The restrictions on \( M \) and \( L \) can be easily verified by substituting (29) and (30) in (27). Eliminating \( f_t \) from (30) with the help of (29) we get the governing kinetic law for normal velocity of the GB:

\[
V = \frac{ML}{L + M\beta^2} f + \frac{M\beta}{L + M\beta^2} \dot{C}, \quad (31)
\]

where the homogeneous translational velocity \( \dot{C} \) is to be obtained by using (30) and (28) in (29) and then integrating it over \( \mathcal{C} \):

\[
\dot{C} = \frac{\int_{\mathcal{C}} \left( \frac{M\beta}{L + M\beta^2} f + \tau n \cdot e_2 \right) dl}{\int_{\mathcal{C}} \left( \frac{1}{L + M\beta^2} + \frac{\rho I}{D} n \cdot e_1 - \frac{y^2}{D} \right) dl}. \quad (32)
\]

Solving (31) and (32) simultaneously we can determine the updated location of the GB as well as of the center of mass of the upper grain. According to (32), relative grain translation can occur even in the absence of external stress. The magnitude of sliding will however be small as the sliding rate is proportional to the integral of the curvature (which continuously changes sign) over the entire GB (assuming the GB energy and the kinetic coefficients to be isotropic). For example, the integral vanishes if the GB is periodic.

As a special case, let’s consider the GB to be planar. Equations (31) and (32) then reduce down to

\[
V = M\beta \tau, \quad \text{and} \quad \dot{C} = (L + M\beta^2) \tau, \quad (33)
\]

respectively. This result is in agreement with the earlier work [23, 27] on low angle tilt GBs where viscous sliding was altogether neglected.

### 3.2 Bicrystal-II

We now consider the 2D bicrystal in Figure 4 (bicrystal-II) where one columnar grain is embedded within another grain. The origin of the coordinate system is such that it coincides with the center of rotation of the embedded grain. Without loss of generality we assume the outer grain to remain stationary while allowing the embedded grain to both rotate and translate with respect to the outer grain. The velocity of the inner grain can be written as

\[
v_1 = \dot{\theta} e_3 \times x + \dot{C}. \quad (33)
\]

Taking a dot product of this relation with \( n = e_3 \times t \) we get

\[
[v_n] = \dot{\theta} x \cdot t + \dot{C} \cdot n. \quad (34)
\]
Earlier MD \cite{31} and PF \cite{34} simulations have confirmed that in the absence of external stress, the embedded grains spontaneously rotates about a fixed center of rotation and shrinks without any translational motion under GB capillary force. Based on this, and considering that the stress amplitude is much smaller than the yield stress, we assume the translational velocity to be much smaller than the rotational velocity. As a result we ignore the effect of translational velocity on GB diffusion and approximately write the mass balance \cite{41} as

\[
\frac{\partial h}{\partial s} = -\rho \dot{\theta} \mathbf{x} \cdot \mathbf{t}.
\]  \quad (35)

Integrating (35), and using the conservation condition \( \oint_{C} h \, dl = 0 \) (which can be easily proved with \cite{19}), we get

\[
h = \frac{\rho \dot{\theta}}{2} (R^2 - \overline{R^2}),
\]  \quad (36)

where \( \overline{R^2} = \oint_{C} R^2\, dl / |C| \) (\(|C|\) stands for the length of \( C \)). Next we substitute from \cite{33}, \cite{34}, and \cite{36} into the dissipation inequality \cite{14} to rewrite it as

\[
fV + g\nu + f_t \cdot \mathbf{C} \geq 0,
\]  \quad (37)

where

\[
g = -\frac{1}{\mathbf{x} \cdot \mathbf{n}} \left( \rho \mu \mathbf{x} \cdot \mathbf{t} + T + \frac{\dot{\theta}}{4D} (R^2 - \overline{R^2})^2 - \frac{\partial \dot{\gamma}}{\partial \theta} \right)
\]  \quad (38)

is the driving force for the rotational velocity \( \nu = \dot{\theta} \mathbf{x} \cdot \mathbf{n}, T = \tau(x_1n_1 - x_2n_2), f_t = \langle \sigma \mathbf{n} \rangle \), and the position vector is expressed as \( \mathbf{x} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 \). In writing \cite{37} we have considered the state of stress as given in \cite{25}. We assume that, while grain rotation and GB migration are coupled with each other, they are both decoupled to grain translation dynamics. The linear kinetic relations can be postulated in the following form: from \cite{37} as

\[
\nu = \beta V + S g,
\]  \quad (39)

\[
V = Mf + M\beta g,
\]  \quad (40)
where \( M > 0, \beta, \) and \( L \geq 0 \) have the same meaning as before; \( S \geq 0 \) denotes the isotropic grain rotational sliding coefficient. These kinetic relations are consistent with the recent MD and PF studies \([31, 32, 34]\) where no grain translation was reported during the coupled motion under GB capillary force in the absence of stress. Equations \((39)\) and \((40)\) are the kinetic relations for GB velocity and grain rotation \([2, 5]\), whereas \((41)\) is an additional kinetic equation for the translational velocity of the embedded grain. Replacing \( g \) in \((40)\) from \((39)\) we derive an equation for the normal velocity of the GB \([2, 30]\)

\[
\dot{V} = \frac{MS}{S + M\beta^2} f - \frac{M\beta}{S + M\beta^2} \dot{\theta} \mathbf{x} \cdot \mathbf{n}.
\]  

(42)

On the other hand, using \((40)\) and \((38)\) in \((39)\) and then integrating it over the entire GB \(\mathcal{C}\) we obtain

\[
\dot{\theta} = \frac{-\int_{\mathcal{C}} \left( \frac{M\beta}{S + M\beta^2} f \mathbf{x} \cdot \mathbf{n} + \frac{\partial \gamma}{\partial \theta} - T \right) dl}{\int_{\mathcal{C}} \left( \frac{(\mathbf{x} \cdot \mathbf{n})^2}{S + M\beta^2} - \frac{1}{2D(R^2 - \bar{R}^2)^2} \right) dl}.
\]  

(43)

The translational velocity of the grain \(\dot{\mathbf{C}}\), which is homogeneous in its domain, is computed by integrating \((44)\) over the closed curve:

\[
\dot{\mathbf{C}} = \frac{\tau L}{|\mathcal{C}|} \int_{\mathcal{C}} (n_2 e_1 + n_1 e_2) dl.
\]  

(44)

Equations \((42)\), \((43)\), and \((44)\) have to be solved simultaneously to obtain the new GB position, grain orientation, and the location of the center of mass of the embedded grain. It is straightforward to note from \((44)\) that if the GB is symmetric about both \(e_1\) and \(e_2\)-axes, for e.g. having a circular or an elliptic shape, there will not be any translation of the embedded grain under the present state of stress. This is in agreement with the finding of Cahn and Taylor \([5]\) where the applied stress was considered just to assist in the rotation while no translational motion of the embedded grain was considered. If the shape of \(\mathcal{C}\) is asymmetric, the stress sets the embedded grain into translation. Despite many simplifying approximations made on the nature of kinetics, our model is capable of capturing the essential physics of the phenomena. In absence of the external stress, we recover the same kinetic relations for GB motion and grain rotation as derived earlier in \([2,30]\).

### 3.3 Tricrystal

We now derive kinetic relations for a 2D tricrystal subjected to shear stress as shown in Figure 5. The tricrystal configuration consists of three grains \(G_1, G_2,\) and \(G_3\), four boundaries \(\mathcal{C}_i, i = 1, \ldots, 4\), and two junctions \(J_1\) and \(J_2\). Orientation of the respective grains, denoted by \(\psi_1, \psi_2,\) and \(\psi_3\) (measured anticlockwise w.r.t. the \(e_1\)-axis), are considered to be homogeneous (since they are all rigid and defect free). The tricrystal lies in a plane (spanned by \(e_1\) and \(e_2\)) orthogonal to \(e_3\), where \(\{e_1, e_2, e_3\}\) forms a right-handed orthonormal basis. The origin of the coordinate system is taken to coincide with the center of rotation of \(G_1\). Since we assume that the tricrystal is initially symmetric about \(e_2\)-axis, and
also that the external loading is symmetric about the same axis, the instantaneous rotational velocity of two points in $G_1$ located in the neighborhood of $J_1$ and $J_2$ will always be equal and opposite until $G_1$ disappears. As a consequence, the mid-point of the line joining $J_1$ and $J_2$ will throughout represent the center of rotation, where the rotation axis is parallel to $e_3$. Thus $\{e_1, e_2, e_3\}$ represent a basis for the translating coordinate with the origin held fixed with the instantaneous center of rotation. The misorientation angles along $C_1, C_2,$ and $C_{3,4}$ are defined as $\theta_1 = \psi_1 - \psi_2$, $\theta_2 = \psi_1 - \psi_3$, and $\theta_3 = \psi_2 - \psi_3$, respectively. The arc-length parameter for $C_i$ is denoted by $s_i$ ($i = 1, \ldots, 4$) with an increasing direction as shown in Figure 5. The normal $n_i$ and the tangent $t_i$ for a GB $C_i$ is also shown in the same figure, where the latter is aligned in the direction of increasing $s_i$. The state of stress in each of the grains is assumed to be given by (25), which trivially satisfies the equilibrium equations and the traction boundary conditions. Let $R_i(\phi, t)$ be the radial distance of the GB $C_i$ from the center of rotation $O$ measured at an angle $\phi_i$ w.r.t. $e_1$-axis (see Figure 5), where $0 \leq \phi_1 \leq \pi$ and $\pi \leq \phi_2 \leq 2\pi$. Denote the position vectors for the junctions $J_1$ and $J_2$ by $z_1$ and $z_2$, respectively and the position vectors of the edges $Q_1$ and $Q_2$ by $z_3$ and $z_4$, respectively.

We allow the embedded grain $G_1$ to both rotate and translate with respect to the neighboring grains. The outer grains $G_2$ and $G_3$ are however restricted to undergo only relative translational motion. This is consistent with the observations made through MD simulations in [32]. Without loss of generality we assume that $G_3$ remains stationary. Hence, $\dot{\theta}_1 = \dot{\theta}_2 = \dot{\psi}_1$ and $\dot{\theta}_3 = 0$. Based on these assumptions, the velocity of the three grains take the form

$$v_1 = \dot{\psi}_1 e_3 \times \mathbf{x} + \dot{C}_1, \quad v_2 = \dot{C}_2, \quad v_3 = 0,$$

(45)

where $C_1$ and $C_2$ are the rigid translations of $G_1$ and $G_2$, respectively. Define vectors $C_1 = C_1 - C_2$, $C_2 = C_1$ and $C_{3,4} = C_2$, as representing the relative translation between the adjacent grains across $C_1$, $C_2$, and $C_{3,4}$, respectively. The normal and the tangent vector for $C_a$ (from now on suffix $a$ will stand

Figure 5: A schematic of the tricrystal.
for either 1 or 2, and suffix $b$ for either 3 or 4) can be written as

$$n_a = -\frac{(R_a\cos\phi_a - R'_a\sin\phi_a)}{\sqrt{R_a^2 + R'_a^2}}e_1 - \frac{(R_a\sin\phi_a + R'_a\cos\phi_a)}{\sqrt{R_a^2 + R'_a^2}}e_2, \quad (46)$$

$$t_a = (n_a \cdot e_2)e_1 - (n_a \cdot e_1)e_2, \quad (47)$$

respectively (no summation for the repeated index $a$), where $R'_a = \partial R_a/\partial \phi_a$. Using $n_a = e_3 \times t_a$ the normal component of the velocity $v_1$, when evaluated on $\mathcal{C}_1$ and $\mathcal{C}_2$, yields

$$v_1 \cdot n_1 = \dot{\psi}_1 x \cdot t_1 + \dot{C}_1 \cdot n_1 \quad \text{and} \quad v_1 \cdot n_2 = \dot{\psi}_1 x \cdot t_2 + \dot{C}_1 \cdot n_2, \quad (48)$$

respectively. The relative tangential velocities at $\mathcal{C}_1$, $\mathcal{C}_2$, and $\mathcal{C}_{3,4}$, defined as $\nu_1 = (v_1 - v_2) \cdot t_1$, $\nu_2 = (v_1 - v_3) \cdot t_2$, and $\nu_{3,4} = (v_2 - v_3) \cdot t_{3,4}$, can be computed using (45) as (no summation for the index $b$)

$$\nu_a = -\dot{\psi}_1 x \cdot n_a + \dot{C}_a \cdot t_a \quad \text{for} \quad a = 1, 2 \quad \text{and} \quad \nu_b = \dot{C}_b \cdot t_b \quad \text{for} \quad b = 3, 4. \quad (49)$$

**Consequence of mass balance** Following our discussion in Section 3.2 we ignore the role of the translational balance in the mass balance relation in comparison with its rotational counterpart. Henceforth using (45) and (48) in (4) we rewrite the mass balance at the GBs as

$$\frac{\partial h_a}{\partial s_a} = -\rho \dot{\psi}_1 x \cdot t_a \quad \text{on} \quad \mathcal{C}_a \quad \text{and} \quad \frac{\partial h_b}{\partial s_b} = -\rho \dot{C}_2 \cdot n_b \quad \text{on} \quad \mathcal{C}_b. \quad (50)$$

Expanding (5) we obtain the following conditions for the diffusion currents at the junctions:

$$h_1 - h_2 - h_4 = 0 \quad \text{at} \quad J_1 \quad \text{and} \quad h_1 - h_2 + h_3 = 0 \quad \text{at} \quad J_2, \quad (51)$$

Substituting from (46) and (47) into (50), while recalling that $n_b = (-1)^{b-1}e_3 \times t_b$, and integrating the result yields

$$h_a = \frac{\rho \dot{\psi}_1}{2}R_a^2 + k_a \quad \text{and} \quad h_b = (-1)^{b-1}\rho \dot{C}_2 \cdot e_3 \times x_b + k_b, \quad (52)$$

where $k_a$ and $k_b$ are the integration constants, and $x_b = x(s_b)$. Since the tricrystal has been assumed not to exchange mass with the surrounding, $h_b$ must satisfy $h_3(z_3) = 0$ and $h_4(z_4) = 0$. With these boundary conditions, (52) simplifies to

$$h_b = (-1)^{b-1}\rho \dot{C}_2 \cdot e_3 \times (x_b - z_b). \quad (53)$$

The GBs $\mathcal{C}_3$ and $\mathcal{C}_4$ are always symmetrically equivalent about $e_2$-axis, hence the validity of (53) for both these curves demands that $\dot{C}_2$ must be parallel to $e_1$, i.e. $\dot{C}_2 = \dot{C}_2e_1$, which implies that the
upper grain will always move in a horizontal direction with respect to the lower grains. Consequently, (53) reduces down to
\[ h_b = (-1)^{b-1} \rho \dot{C}_2 y_b, \]  
where \( y_b = (x_b - z_b) \cdot e_2 \).

Using (52) and (53) in (51) and neglecting the contribution coming from the translational velocity in comparison to the rotational speed as far as the diffusion fluxes along \( \mathcal{C}_1 \) and \( \mathcal{C}_2 \) are concerned, we conclude that
\[ k_1 - k_2 = 0 \text{ at } J_1 \text{ and } J_2. \]  

Equations (53) and (52) in association with the conservation condition \( \int_{\mathcal{C}_1} h_1 \, dl + \int_{\mathcal{C}_2} h_2 \, dl = 0 \) along the closed boundary of \( G_1 \) yield
\[ h_a = \frac{\rho \dot{\psi}_1}{2} (R^2 - \overline{R}^2), \]  
where \( \overline{R}^2 = (\int_{\mathcal{C}_1} R_1^2 \, dl + \int_{\mathcal{C}_2} R_2^2 \, dl)/(|\mathcal{C}_1| + |\mathcal{C}_2|) \). The conservation condition can be easily proved using the Fick’s law (19). Moreover, applying (19) in (54) and then integrating the equation we get the chemical potential along \( \mathcal{C}_b \) as
\[ \mu_b = (-1)^b \frac{\rho \dot{C}_2}{D_b} I_b, \]  
where the chemical potential at the free surfaces has been considered to be zero as discussed in Section 3.1 and \( I_b = \int_{s_b(z_b)}^{y_b} y_b \, dl \).

**Kinetic relations** At first we derive the kinetic laws related to the dynamics of \( \mathcal{C}_a \) and \( G_1 \), and then move on to the kinetics of the other GBs and junctions. Ignoring the terms of the order of \( \dot{\mathcal{C}}_a \dot{\psi}_1 \) and \( \dot{\mathcal{C}}_a^2 \), while using (7), (43), (48), and (19) in (14), we rewrite the dissipation inequality on \( \mathcal{C}_a \) as
\[ f_a V_a + g_a \nu_a + \sigma_a \dot{\mathcal{C}}_a \geq 0 \text{ on } \mathcal{C}_a, \]  
where
\[ g_a = \frac{1}{x_a \cdot n_a} \left( \frac{\partial \gamma_a}{\partial \theta_a} - \rho \mu_a x_a \cdot t_a - \frac{\dot{\psi}_1}{4 D_a} (R_a^2 - \overline{R}_a^2)^2 - T_a \right) \]  
is the driving force for the rotational motion of \( G_1 \) with
\[ T_a = \tau ((n_a \cdot e_1)(x_a \cdot e_1) - (n_a \cdot e_2)(x_a \cdot e_2)); \]  
\( \nu_a = -\dot{\psi}_1 x_a \cdot n_a \) is related to the rotational velocity of \( G_1 \); \( \sigma_a = \langle \sigma n_a \rangle \cdot e_1 = \tau n_a \cdot e_2 \) is the driving force for the translational motion between the adjacent grains; and \( \dot{\mathcal{C}}_a = (\dot{\mathcal{C}}_1 - \dot{\mathcal{C}}_2) \cdot e_1 \). While deriving (58) we have neglected a term proportional to \( \mu_a \dot{\mathcal{C}}_a \), which is estimated to be of the order of \( \dot{\psi}_1 \dot{\mathcal{C}}_a + \dot{\mathcal{C}}_a^2 \) considering (19) and (56). The term \( \sigma_a \dot{\mathcal{C}}_a \) in (59) is derived from what originally was of the form \( \langle \sigma n_a \rangle \cdot \dot{\mathcal{C}}_a \). Indeed, the tricrystal will always maintain the symmetry (about \( e_2 \)-axis) as dictated by its initial geometry and the loading condition. Moreover, since the relative velocities \( \dot{\mathcal{C}}_a \) are uniform over the respective GBs, we can justifiably assume that it is only the average values of their conjugate forces, i.e. \( \int_{\mathcal{C}_a} \tau (n_2 e_1 + n_1 e_2) \, dl / |\mathcal{C}_a| \), which are ultimately going to contribute to the net dissipation.
Assuming linear kinetics, and recalling the Onsager’s reciprocity theorem \cite{25}, we consider the following set of phenomenological kinetic equations for the fluxes on $C_a$ \cite{2,5}:

\begin{align}
V_a &= M_a f_a + M_a \beta_a g_a, \tag{60} \\
\nu_a &= \beta_a V_a + S_a g_a, \tag{61} \\
\dot{\gamma}_a &= L_a \sigma_a, \tag{62}
\end{align}

where $M_a > 0$, $\beta_a$, $S_a \geq 0$, and $L_a \geq 0$ have the same meaning as discussed earlier. For the same reason as discussed in Section 3.2, we assume the translational velocity of the embedded grain to be decoupled from rotation evolution and migration. Multiplying both sides of (60) by $S_a$ and then replacing $g_a$ from it using (61) we get

\begin{align}
V_a &= M_a S_a + M_a \beta_a \left( f_a + \beta_a \nu_a \right), \tag{63}
\end{align}

which is the governing equation for normal velocity of $C_a$. To calculate $\dot{\psi}_1$ we begin by combining (60) with (61), after replacing $g_a$ from (59), to obtain

\begin{align}
\dot{\psi}_1 \left( \frac{(x_a \cdot n_a)^2}{S_a + M_a \beta_a^2} - \frac{1}{4D_a} (R_a^2 - \bar{R}_a^2)^2 \right) &= - \frac{M_a \beta_a}{S_a + M_a \beta_a^2} (x_a \cdot n_a) f_a - \frac{\partial \gamma_a}{\partial \theta_a} + T_a + \mu_a x_a \cdot t_a. \tag{64}
\end{align}

These two equations (for $a = 1, 2$) are then integrated over $C_1$ and $C_2$, respectively, and summed up to write the ordinary differential equation

\begin{align}
\dot{\psi}_1 &= - \sum_{a=1}^{2} \int_{C_a} \left( \frac{M_a \beta_a}{S_a + M_a \beta_a^2} f_a x_a \cdot n_a + \frac{\partial \gamma_a}{\partial \theta_a} - T_a \right) dl, \tag{65}
\end{align}

where we have used the identity (obtained using (19) and (56))

\begin{align}
\sum_{a=1}^{2} \int_{C_a} \mu_a x_a \cdot t_a dl = \frac{2}{4D_a} (R_a^2 - \bar{R}_a^2)^2 dl. \tag{66}
\end{align}

Note that (65) coincides with (43) for bicrystal-II when junctions are ignored. We now have the kinetic relations corresponding to the normal velocities of $C_1$ and $C_2$ in (63), and the rotational speed of the inner grain $G_1$ in (65). In the following we will derive kinetics for the normal velocity of boundaries $C_3$ and $C_4$, the translational velocity of the grains $G_1$ and $G_2$, and the velocities for $J_1$ and $J_2$.

The dissipation inequality (14) for the GBs $C_3$ and $C_4$, across which there is no misorientation evolution, can be reduced to

\begin{align}
f_b V_b + \sigma_b (\dot{C}_2)_b \geq 0, \tag{66}
\end{align}

where

\begin{align}
\sigma_b = (-1)^b \frac{(\dot{C}_2)_b}{D_b} f_b n_b \cdot e_1 + \tau n_b \cdot e_2 + \frac{\rho^2}{D_b} (\dot{C}_2)_b y_b^2. \tag{67}
\end{align}
As done previously we postulate linear kinetics from (66):

\[
(\dot{C}_2)_b = \beta_b V_b + L_b \sigma_b, \tag{68}
\]

\[
V_b = M_b f_b + M_b \beta_b \sigma_b. \tag{69}
\]

Eliminating \(\sigma_b\) between (69) and (68) we obtain the governing kinetic law for normal velocity of \(C_b\)

\[
V_b = \frac{M_b L_b}{L_b + M_b \beta_b^2} f_b + \frac{M_b \beta_b}{L_b + M_b \beta_b^2} (\dot{C}_2)_b. \tag{70}
\]

To derive an expression for the translational velocity of \(G_2\) we substitute \(V_b\) from (69) into (68), then integrate it over \(C_3\) and \(C_4\), respectively for \(b = 3, 4\), and finally add them up to obtain

\[
\dot{C}_2 = \frac{\sum_{b=3}^{4} \int_{\varphi_b} \left( \frac{M_b \beta_b}{L_b + M_b \beta_b^2} f_b + \tau n_b \cdot e_2 \right) dl}{\sum_{b=3}^{4} \int_{\varphi_b} \left( \frac{1}{L_b + M_b \beta_b^2} - (-1)^b \frac{I_b}{D_b} n_b \cdot e_1 - \frac{1}{D_b} \bar{y}_b^2 \right) dl}. \tag{71}
\]

Next we integrate (62) respectively for \(a = 1\) and \(2\), and combine them to obtain the average of the translational velocity of \(G_1\) as

\[
\dot{C}_1 = \frac{1}{|C_1| + |C_2|} \left( \dot{C}_2 |C_1| + \sum_{a=1}^{2} \int_{\varphi_a} L_a \sigma_a dl \right). \tag{72}
\]

We now have all the required kinetic relations related to GB motion and grain dynamics.

In rest of this section, we will focus our attention to derive the kinetic relations for the two junctions. Considering a weak singularity in stress, as discussed in 2.2, one can show that the closed integral in (15) would vanish in the limit \(\epsilon \to 0\). Linear kinetic relations can then be motivated from the reduced dissipation inequality at the junctions as \[9\]

\[
q_{\delta} = m_{\delta} F_{\delta} \text{ at } J_{\delta} \text{ for } \delta = 1, 2
\]

where \(m_{\delta} \geq 0\) is the mobility coefficient associated with junction \(J_{\delta}\),

\[
F_1 = \gamma_1 t_1 - \gamma_2 t_2 - \gamma_4 t_4, \text{ and } \tag{74}
\]

\[
F_2 = -\gamma_1 t_1 + \gamma_2 t_2 - \gamma_3 t_3. \tag{75}
\]

We assume the junctions to be non-splitting. Compatibility at the junctions would then require \[9\]

\[
V_i = q_1 \cdot n_i \text{ at } J_1 \text{ for } i = 1, 2, 4, \tag{76}
\]

\[
V_i = q_2 \cdot n_i \text{ at } J_2 \text{ for } i = 1, 2, 3. \tag{77}
\]

These compatibility equations will be used to determine the junction angles, as described below.

It follows from the geometry of the tricrystal that

\[
n_i \cdot t_j = \sin(\alpha_j - \alpha_i) \text{ and } t_i \cdot t_j = \cos(\alpha_i - \alpha_j) \text{ for } i, j = 1, 2, 3, 4
\]
at the junctions, where $\alpha_i$ is the angle made by the tangent (in the limiting sense) to $C_i$ with $e_1$-axis at the corresponding junction (see Figure 5). Substituting $F_\delta$ from (74) and (75), using (73), in (76) and (77), and then employing (78) in the resulting relations we obtain the following sets of compatibility relations:

$$-\gamma_2 \sin(\alpha_2 - \alpha_1) - \gamma_4 \sin(\alpha_4 - \alpha_1) = \frac{V_1}{m_1},$$  

$$\gamma_1 \sin(\alpha_1 - \alpha_2) - \gamma_4 \sin(\alpha_4 - \alpha_2) = \frac{V_2}{m_1},$$  

$$\gamma_1 \sin(\alpha_1 - \alpha_4) - \gamma_2 \sin(\alpha_2 - \alpha_4) = \frac{V_4}{m_1} \text{ at } J_1, \text{ and}$$  

$$\gamma_2 \sin(\alpha_2 - \alpha_1) - \gamma_3 \sin(\alpha_3 - \alpha_1) = \frac{V_1}{m_2},$$  

$$-\gamma_1 \sin(\alpha_1 - \alpha_2) - \gamma_3 \sin(\alpha_3 - \alpha_2) = \frac{V_2}{m_2},$$  

$$-\gamma_1 \sin(\alpha_1 - \alpha_3) + \gamma_2 \sin(\alpha_2 - \alpha_3) = \frac{V_3}{m_2} \text{ at } J_2,$$  

(79)

(80)

when $m_\delta > 0$. The nonlinear algebraic equations given by (79) and (80) have to be solved in order to obtain $\{\alpha_1, \alpha_2, \alpha_4\}$ and $\{\alpha_1, \alpha_2, \alpha_3\}$ at $J_1$ and $J_2$, respectively. Using (74) and (75) in (73) the junction velocities are calculated as

$$q_1 = m_1(\gamma_1 \cos \alpha_1 - \gamma_2 \cos \alpha_2 - \gamma_4 \cos \alpha_4)e_1 + m_1(\gamma_1 \sin \alpha_1 - \gamma_2 \sin \alpha_2 - \gamma_4 \sin \alpha_4)e_2 \text{ and}$$  

$$q_2 = m_2(-\gamma_1 \cos \alpha_1 + \gamma_2 \cos \alpha_2 - \gamma_3 \cos \alpha_3)e_1 + m_2(-\gamma_1 \sin \alpha_1 + \gamma_2 \sin \alpha_2 - \gamma_3 \sin \alpha_3)e_2. \quad (81)$$

When the junction mobility is infinite, i.e. $m_\delta \to \infty$, (79) and (80) give two independent equations

$$\frac{\gamma_1}{\sin(\alpha_2 - \alpha_4)} = \frac{\gamma_2}{\sin(\alpha_1 - \alpha_2)} = \frac{-\gamma_4}{\sin(\alpha_1 - \alpha_2)} \text{ at } J_1 \text{ and}$$  

$$\frac{\gamma_1}{\sin(\alpha_2 - \alpha_3)} = \frac{-\gamma_2}{\sin(\alpha_3 - \alpha_1)} = \frac{\gamma_3}{\sin(\alpha_1 - \alpha_2)} \text{ at } J_2,$$  

(82)

(83)

known as the Young-Dupré equations [9]. In order to solve the junction angles uniquely, we use the following equations which are obtained by eliminating $m_1$ and $m_2$ from the respective sets of equations from (79) and (80):

$$\gamma_1 V_1 - \gamma_2 V_2 - \gamma_3 V_3 = 0 \text{ at } J_1 \text{ and } \gamma_1 V_1 - \gamma_2 V_2 + \gamma_4 V_4 = 0 \text{ at } J_2.$$  

(84)

To calculate the velocity of $J_1$ when $m_1 \to \infty$, we consider $q_1 = q_1(\cos \xi e_1 + \sin \xi e_2)$ where $\xi$ is the angle made by $q_1$ with $e_1$-axis. Using this expression in (76) twice (i.e. for two different values of $i$) we get

$$q_1 = \csc(\alpha_j - \alpha_i) ((V_i \cos \alpha_j - V_j \cos \alpha_i)e_1 + (V_i \sin \alpha_j - V_j \sin \alpha_i)e_2) \text{ for any } i, j = 1, 2, 4, \text{ } i \neq j. \quad (85)$$

The expression for the velocity of $J_2$ is exactly same as (85), except the indices are now restricted to $i, j = 1, 2, 3$.  

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To summarize, the migration kinetics of GBs $C_1$ and $C_2$ is governed by (63), which is a non-linear parabolic partial differential equation, whereas GBs $C_3$ and $C_4$ migrate following (70). Equations (65), (71), and (72) govern the homogeneously evolving orientation for $G_1$, the uniform horizontal translation for $G_2$, and uniform horizontal translation for $G_1$, respectively, while keeping the grain $G_3$ fixed. The junction dynamics at $J_1$ and $J_2$ follows (81) when the mobility coefficient is of finite magnitude. The unknown junction angles $\alpha_1$, $\alpha_2$, and $\alpha_3$ at $J_1$ and $J_2$ are obtained by solving the set of equations in (79) and (80), respectively. The junction motion is governed by (85) when the mobility coefficient takes an infinite value, and the three unknown junction angles are then determined by solving (82), (83), and (84) for $J_1$ and $J_2$ as indicated in the respective equations. In the absence of junctions, for instance when $G_2$ and $G_3$ are identical grains, the kinetic relations (63) and (65) reduce to a form derived in [2, 30].

4 Constitutive assumptions

Before proceeding towards numerical simulations we fix the constitutive form of GB energy and various kinetic coefficients. We assume that the GB energy $\gamma$, the coupling factor $\beta$, and the kinetic coefficients $M$, $S$, and $L$ are all isotropic, and hence functions of only the misorientation angle at the GB (denoted by $\theta$). We will in fact assume the mobility, the sliding, and the translating coefficients to remain constant, writing them as $M = M_0$, $S = S_0$, and $L = L_0$, respectively. The GB energy is written as $\gamma = \gamma_0 \tilde{\gamma}(\theta)$, where $\gamma_0$ is a constant. The junction mobility coefficient, assumed to be same for both $J_1$ and $J_2$, has also been taken as a constant.

4.1 GB energy

The analytical model for the energy of low angle GBs, initially proposed by Read and Shockley [27], has been extended to high angle GBs by several researchers [24, 28]. Here we will use the form of GB energy as derived from a disclination model of GB [24, 28]. The expression of energy density thus obtained is valid for the entire range of misorientation angles, unlike the forulma obtained from the dislocation based model of GB. It is given by

$$\tilde{\gamma}(\theta) = \begin{cases} (\theta - \theta_A) [A_c - \ln(\theta - \theta_A)] , & \text{for } \theta_A \leq \theta \leq \theta_c , \\ (\gamma_1 - \gamma_2) \left( 1 - \frac{\theta - \theta_A}{\theta_B - \theta_c} \right) + (\theta_B - \theta) \left( A_c - \ln(\theta_B - \theta) \right) , & \text{for } \theta_c \leq \theta \leq \theta_B , \end{cases}$$

(86)

where

$$A_c = \ln \left( \frac{\exp(3/2)(\theta_B - \theta_A)}{2\pi} \right).$$

(87)

For a (100) symmetric tilt boundary in cubic crystals, $\theta_A = 0$ and $\theta_B = \pi/2$. The angle $\theta_c$ represents the misorientation angle where $\gamma$ has a cusp; we take it as 36.9°. The term $\gamma_1$ is given by $\tilde{\gamma}$, evaluated at $\theta_c$, using the first expression in (86), whereas $\gamma_2$, also evaluated from $\tilde{\gamma}$ at $\theta_c$, but after replacing $\theta - \theta_A$ by $\theta_B - \theta$ in the first expression for $\tilde{\gamma}$ in (86). It is to be noted that (86) coincides with Read-Shockley energy in the small misorientation range ($\theta < 15^\circ$). A plot of the energy, smoothened at its cusp, is shown in Figure 6(a).
4.2 Geometric coupling factor

An analytical form for the geometric coupling factor $\beta$ was first derived by Cahn et al. [3]. They considered shear coupled motion in a bicrystal with a planar low angle symmetric tilt boundary where, subjected to shear stress parallel to the GB, the bicrystal experiences a simple shear deformation in the region swept by the GB. The coupling factor, defined as the ratio of the relative tangential velocity of the grains at the GB to the normal speed of the boundary, was obtained as $\beta(\theta) = 2\tan(\theta/2)$. For small misorientation this expression for the coupling factor agrees with that used by Read and Shockley [27]. Further investigation has shown that $\beta$ can in fact suffer a jump discontinuity at a specific misorientation angle (we denote it by $\theta_\beta$) resulting in a shift of GB dynamics from one mode to another [4]. The modified form of the coupling factor is [3]

$$\beta(\theta) = \begin{cases} 
2\tan(\theta/2) & \text{for } 0 \leq \theta \leq \theta_\beta, \\
-2\tan(\pi/4 - \theta/2) & \text{for } \theta_\beta < \theta \leq 90^\circ,
\end{cases} \quad (88)$$

where the two functions are referred to as the coupling modes of $\langle 100 \rangle$ and $\langle 110 \rangle$ types, respectively. The expression for coupling factor was experimentally verified by Gottstein and coworkers [23] for both low angle and high angle planar boundaries. More recently, MD simulations [31] have confirmed that the coupling factor (88), as well as the phenomena of mode shifting, remains applicable during the coupled motion of curved GBs. We will adopt (88) for the simulations in the following section with $\theta_\beta = 36.9^\circ$ [31]. Figure 6(b) shows the plot of (88) in addition to its smoothened version. Suitable smoothening of singularities in both GB energy and coupling factor is necessary for our computational framework such that the kinetic relations for GBs, grain orientations, and junctions remain well-posed.

5 Results and discussion

We introduce non-dimensional position and time variables as $\tilde{x} = x/R_0$ and $\tilde{t} = t/t_0$, respectively, where $t_0 = R_0^2/2\gamma_0 M_0$ is the time taken for an isolated circular GB of radius $R_0$, with energy $\gamma_0$.
and mobility $M_0$, to vanish under curvature driven migration. These dimensionless variables can be substituted in (63), (70), (65), (72), (71), and (80)–(85), to obtain a system of non-dimensionalized kinetic equations for the tricrystal. The non-dimensionalized version of equations (83) and (84) for bicrystal-I, and (12)–(14) for bicrystal-II can be obtained similarly. This naturally introduces three dimensionless parameters $r_1 = S_0/M_0$, $r_2 = M_0R_0^2/D$, and $r_3 = L_0/M_0$ associated with GB kinetics, and one non-dimensional parameter $\Lambda_δ = 2\rho_0m_δ/M_0$ with junction kinetics [2, 8]. We restrict our simulations to constant mobility, sliding coefficients, and translation coefficient assumed to be same for all the GBs, and also constant junction mobility coefficient, considered same for both the junctions. Hence, say $\Lambda_1 = \Lambda_2 = \Lambda$. The value of the dimensionless parameters are taken as $0.01 \leq r_1 \leq 1$, $r_2 = 10^3R(0)/R(t))^{3/2}$, and $1 \leq \Lambda \leq \infty$ [2, 8]. The time-dependent term in $r_2$ ensures that with decreasing grain size GB diffusivity increases [7]. Because of lack of proper data related to the translational coefficient $L_0$, we consider $r_3 = 1$ (unless we specify a different value) in order to observe tangible grain translations. All the parameters have been taken for face-centered cubic crystals.

The non-dimensionalized kinetic equations are solved numerically to investigate the shape and orientation evolution of the embedded grain. Our simulation methodology is based on the finite difference scheme proposed by Fischer et al. [9]. The scheme is described briefly for the tricrystal; it simplifies for bicrystal-II in a straightforward manner. The GB $G_i$ (recall that the subscript $i$ refers to one of the GBs in the tricrystal arrangement) has been discretized with $N_i$ number of grid points (discretization goes in the direction of increasing $s_i$) with the position vector (non-dimensionalized) denoted by $\tilde{x}_i^j = x_i^j e_1 + y_i^j e_2$, where the superfix $j = 0, \ldots, N_i$ denotes the index of the grid points on $G_i$. The position of the grid points of $G_a$ and $G_b$ are updated at time instance $\tilde{t}_{n+1}$ using the following explicit time integration scheme (superposed tilde represents dimensionless variables):

$$\tilde{x}_a^j(\tilde{t}_{n+1}) = \tilde{x}_a^j(\tilde{t}_n) + \Delta \tilde{t} \tilde{V}_a^j(\tilde{t}_n) \tilde{n}_a^j(\tilde{t}_n) + \Delta \tilde{t} \tilde{C}_1 \tilde{e}_1, \quad \text{for } j = 1, \ldots, N_a - 1,$$

$$\tilde{x}_b^j(\tilde{t}_{n+1}) = \tilde{x}_b^j(\tilde{t}_n) + \Delta \tilde{t} \tilde{V}_b^j(\tilde{t}_n) \tilde{n}_b^j(\tilde{t}_n), \quad \text{for } j = 1, \ldots, N_b - 1,$$

where $\Delta \tilde{t}$ is the time step, $\tilde{V}_a^j$ and $\tilde{V}_b^j$ are the velocity of $G_a$ and $G_b$ given by the non-dimensionalized versions of (63) for $a = 1, 2$ and (70) for $b = 3, 4$. Details of the discretization for $\tilde{R}_0^j$, $\tilde{n}_a^j$ etc. can be seen from [9]. The Rectangle rule for integration has been used in (65), (72), and (71) to compute the non-dimensional rotation rate and the translation rate of grains $G_1$ and $G_2$, respectively. The end point velocities $\tilde{V}_i^{N_i}$ and $\tilde{V}_i^{N_i}$, which are used to compute the junction angles, are computed following [9]. The position vector $\tilde{x}_δ$ of $J_δ$ is updated using

$$\tilde{x}_δ(\tilde{t}_{n+1}) = \tilde{x}_δ(\tilde{t}_n) + \Delta \tilde{t} (\tilde{q}_δ(\tilde{t}_n) + \tilde{C}_1 \tilde{e}_1).$$

where $\tilde{q}_δ$ is given by the non-dimensional version of (81) when the junction mobility is finite and by (85) when the mobility is infinite.

We now present the simulation results for bicrystal-II and tricrystal arrangements. At first, we ignore the external stress and study GB capillary driven dynamics. Next we incorporate the effect of applied shear stress and compare the results with those obtained without it. We consider a bicrystal where the embedded grain has an asymmetric shape; we discretize the GB initially with $N = 100$ grid
Figure 7: Shape evolution under GB migration when \( r_1 = 0.01, \psi_1 = 14^\circ, \psi_2 = 0^\circ, \) and \( \psi_3 = 60^\circ. \) Rows (i) to (iii) correspond to \( \Lambda \to \infty, \Lambda = 20, \) and \( \Lambda = 1, \) respectively.

Figure 8: Shape evolution under fully coupled GB motion when \( r_1 = 0.01, \) and initial \( \psi_1 = 14^\circ, \psi_2 = 0^\circ \) and \( \psi_3 = 60^\circ. \) Rows (i) to (iii) correspond to \( \Lambda \to \infty, \Lambda = 20, \) and \( \Lambda = 1, \) respectively.

points. The Initial misorientation is taken to be \( 8^\circ. \) For the tricrystal we choose the initial discretization of the curved GBs as \( N_a = 100 \) and the planar GBs as \( N_{3,4} = 50 \) grid points. The embedded grain \( G_1 \) is initially taken to be circular with radius \( \tilde{R}_a(0) = 0.4. \) The initial orientation of the grains are taken as \( \psi_1 = 14^\circ, \psi_2 = 0^\circ, \) and \( \psi_3 = 60^\circ. \) The initial misorientations are therefore \( \theta_1 = 14^\circ, \theta_2 = 44^\circ, \) and \( \theta_3 = 30^\circ. \) During the coupled motion, only \( \psi_1 \) (and hence \( \theta_1 \) and \( \theta_2 \)) is allowed to changed while others are kept constant. As a sign convention, if any of the misorientation angles turns out to be negative, we add \( 90^\circ \) to it to obtain an equivalent misorientation angle in the range \( 0 \leq \theta_i < 90^\circ \) recalling that the considered crystals posses a four-fold symmetry [32]. All the computations are done in a domain of size \([-1, 1] \times [-1, 1]\), with time step \( \Delta \tilde{t} \) as \( 10^{-5} \) and \( 10^{-4} \) for the case of GB migration and coupled GB motion, respectively. All the GBs are assumed to be [001] tilt boundaries. To avoid mesh points coming very close to each other or moving far away after time integration, we re-mesh the GBs after every iteration so as to maintain accuracy and stability in all the numerical calculations.
5.1 GB Capillary driven motion

We begin by ignoring the applied stress and restrict our attention to dynamics being driven solely by GB capillary. The translational velocities of the grains are also neglected. We present the results only for the tricrystal since bicrystals with an embedded grain have been extensively studied within the present context [2, 5, 30]. Note that if \( \mathcal{C}_3 \) and \( \mathcal{C}_4 \) are initially planar then they will always remain stationary, i.e. \( V_3 = 0 \) and \( V_4 = 0 \), fixing the junction angles \( \alpha_3 \) and \( \alpha_4 \) for all times. The junction angles \( \alpha_1 \) and \( \alpha_2 \) and the junction velocities in such a situation (where at least one GB at the junction remains stationary) can not be directly calculated using (80)−(85). The pertinent equations can however be easily derived, see e.g. Section 3.3 of [9].

5.1.1 GB migration

With \( \beta \to 0 \) and \( S \to 0 \) the kinetic relations for the tricrystal (63), (70), and (65) are reduced to \( \bar{V}_i = \bar{M}_i \bar{\gamma}_i \bar{\kappa}_i / 2 \) and \( \dot{\psi}_1 = 0 \), respectively. Figure 7 shows the evolution of the embedded grain under these assumptions with both finite and infinite junction mobility. The junction angles start evolving soon after the evolution starts and the embedded grain attains a lens shape. A finite junction mobility drags the GB motion and retards the shrinking rate of the embedded grain. The drag effect increases as \( \Lambda \) decreases and the curved GBs become increasingly flatter before shrinking (see also Figure 9). However, the junction velocities become comparable with those of the GBs when \( \Lambda >> 1 \), which reduces the drag on the GBs. The area evolution then becomes nearly linear and the deviation from linearity increases as \( \Lambda \) decreases. The effect of finite junction mobility has been widely noticed to have a significant influence on GB dynamics (see for e.g. [8]). The drag effects at the junctions are due to frequent dislocation reactions and changes in point defect density in their vicinity (Chapter 3 in [21]).

5.1.2 Coupled GB motion

Depending on the operating conditions, some of the kinetic parameters may be more active than the others. For example, at temperatures near the melting point, viscous GB sliding dominates over geometric coupling, whereas at relatively lower temperatures, sliding is much less active than geometric coupling [3]. We demonstrate the effect of kinetic coefficients on the shape evolution by considering several cases below.

**Fully coupled:** When both sliding and geometric coupling are active, the grain shrinkage becomes much slower than with GB migration alone, as shown in Figures 8 and 9. However, the combined effect of the GB energy and the kinetic coefficients is such that the lower GB shrinks faster than the upper one. The dihedral angles between \( \mathcal{C}_1 \) and \( \mathcal{C}_2 \) are greater in this case than those associated with GB migration at the same time instance (see Figures 7 and 8). The grain \( G_1 \) will disappear after it has shrunk to a vanishing volume leaving a bicrystal in place of the tricrystal. The embedded grain can also disappear, much before it shrinks to a vanishing size, whenever either \( \theta_1 \) or \( \theta_2 \) becomes zero; this is in fact the observed situation in Figure 8 and all other considered simulations except when the motion is uncoupled. We also note that the finite junction mobility not only drags the GB motion, but also
Figure 9: (a) Area and (b) orientation evolution of the embedded grain under normal and coupled GB motion when \( r_1 = 0.01 \). Abbreviations: N - normal GB motion, C - coupled GB motion in absence of \( \beta_1 \) and \( \beta_2 \), and FC - fully coupled GB motion.

slows down the grain rotation, as can be seen in Figure 9(b).

No geometric coupling: In the absence of \( \beta \), the non-dimensional equation for normal velocity reduces down to \( \tilde{V}_a = \tilde{M}_a \tilde{\gamma}_a \tilde{\kappa}_a / 2 \), which is same as the evolution equation for GB migration, except that \( \tilde{\gamma}_a \) is now evolving with time (due to evolving misorientation). Figure 9(a) shows that the area evolution is now slightly slower than the case of GB migration. Orientation \( \psi_1 \) evolves very slowly for most of the time except towards the end. The shape evolution of the curved GBs is nearly identical to the ones shown in Figure 7 for respective junction mobilities. When \( \Lambda \to \infty \) and \( \Lambda = 20 \), the grain shrinks before \( \psi_1 \) could vanish. However, when \( \Lambda = 1 \), \( \psi_1 \) vanishes before the area leaving a bicrystal with a depression on the planar GB, which also eventually vanishes.

No sliding: For \( S \to 0 \) [63] implies that the GB shape, given by \( R_a(\phi_a, t) \), remains self-similar for all times as long as \( \beta \) is isotropic [2, 30]. For example, if \( G_1 \) is initially a circle, then it should remain so for all times during the evolution. Obviously with such a restriction, compatibility equations (79) and (81) or (82), (83), and (84) will have solutions only for very special initial geometries of \( \mathcal{C}_1 \) and \( \mathcal{C}_2 \).

Role of sliding: Higher \( r_1 \) signifies a relative increase of viscous sliding over GB mobility, which is usually seen at elevated temperatures [3]. The rate of change of area and orientation \( \psi_1 \) significantly increases when \( r_1 \) increases as shown in Figures 10(a) and 10(b).

Symmetrically equivalent curved GBs: Let us take orientation \( \psi_3 \) to be \( 28^\circ \) while keeping initial values of \( \psi_1 \) and \( \psi_2 \) same as above. The initial misorientations are therefore \( \theta_1 = 14^\circ \), \( \theta_2 = 76^\circ \), and \( \theta_3 = 62^\circ \). The curved GBs are now symmetrically equivalent with \( \beta_1 = -\beta_2 \). Since the embedded grain is initially symmetric about \( e_1 \)-axis, the first term in the numerator of (65) disappears. However, for the GB energy considered here, the second term in the numerator will always lead to a non-zero rotation of \( G_1 \). On the other hand, if the energy is symmetric about \( \theta = 45^\circ \) (as is the case with the energy given in Figure 6 of [28]), the rotation of \( G_1 \) will vanish and the grain will shrink purely by migration of \( \mathcal{C}_1 \) and \( \mathcal{C}_2 \). This phenomenon of rotation getting locked has been observed in MD [32] and PF simulations [34] when \( \mathcal{C}_1 \) and \( \mathcal{C}_2 \) are symmetrically equivalent.
5.2 Effect of stress on GB dynamics

We now investigate the effect of shear stress $\tau$ on the coupled GB dynamics in the tricrystal shown in Figure 5. We assume that the dynamics is fully coupled. We consider $\tilde{\tau} = 0.1$, which implies that $\tau$ is approximately equal to 10 MPa when $\gamma_0 = 1 \text{ N/m}^2$ and $R_0 = 10 \text{ nm}$. The stress value is much lower than the yield stress which is of the order of few GPa in NC materials [22]. All the other kinetic and geometric data have been kept same as considered above in Section 5.1. Figure 11 shows the evolution of GB, grain, and junction dynamics in the tricrystal. The overall evolution is now slower as compared to that was observed during purely GB capillary driven dynamics in Section 5.1. The center of rotation of the embedded grain can also be seen to translate from the initial position. With increasing junction mobility the magnitude of translation also increases. Figures 12(a) and 12(b) show that decreasing junction mobility marginally increases the rate of grain rotation and grain shrinkage, which is in fact opposite to what has been observed when the dynamics is driven only by GB capillary. This can be attributed to the additional effects coming from the stress related term in (65) and the non-trivial curvature of $C_3$ due to large junction drag when $m_3$ is smaller. All the cases considered in Figure 11 show that vanishing of the misorientation at $C_1$, due to the rotation of the embedded grain, leaves behind a depression on the GB separating the rectangular grains. The depression ultimately disappears so as to eliminate the curvature.

We also have investigated the effect of applied shear stress $\tau$ on shape evolution of the bicrystal arrangement shown in Figure 4. We considered the geometry of $C$ as shown at $\tilde{t} = 0$ in Figure 13. The magnitude of the stress $\tilde{\tau} = 0.1$ considered previously for the tricrystal arrangement does not make any significant difference to the GB dynamics when compared to that observed in the absence of stress. As a result we assume a higher stress $\tilde{\tau} = 30$ (i.e. $\tau = 3 \text{ GPa}$). We take $r_3 = 50$. Figure 13 shows comparison of the shape evolution of the embedded grain when applied stress is absent and when the bicrystal is subjected to shear stress. Clearly the center of rotation of the embedded grain in the latter case is translating, whereas in the former it is fixed.
Figure 11: Shape evolution and dynamics of the embedded grain in the presence of external during fully coupled motion under combined GB capillary force and shear stress of magnitude $\tilde{\tau} = 0.1$ for $\Lambda = 100$ (row(i)), $\Lambda = 20$ (row(ii)), and $\Lambda = 1$ (row(iii)).

Figure 12: A comparative study of (a) area and (b) orientation evolution of the embedded grain during fully coupled motion under shear stress $\tilde{\tau} = 0.1$.

6 Conclusions

We have extended the analytical study of coupled GB motion, hitherto restricted to bicrystals with a columnar grain having a fixed center of rotation embedded in a larger grain, by introducing triple junctions and relative translational sliding in the analysis. The present formulation is applied to bicrystals and tricrystals without restricting the center of rotation of the embedded grain to be fixed. In deriving the necessary kinetic relations we have provided a novel thermodynamic framework within which such and more complicated incoherent interfaces can be studied. Our thermodynamic formalism is closely related to earlier work on incoherent interfaces, most notably [6][13]. The present work can be extended in several directions: i) to analyze the coupled motion in three-dimensions, ii) to include grain deformation in terms of elastic/plastic behaviour of the grains, iii) to include bulk diffusion. While we have considered a simpler case in two-dimensions ignoring these effects, we are still confronted
with a formidable boundary value problem which can be solved satisfactorily only under some further assumptions. For instance when considering anisotropic GB energies a more sophisticated numerical technique (such as the level set method) is needed [2]. However, including junction dynamics within a level set framework remains unsolved except for some very specific cases, restricted to constant interfacial energy and kinetic coefficients along with infinite junction mobility. This led us to consider only isotropic energies so that the resultant problem with junctions is solvable through a simpler numerical scheme. We should also point out that the linear kinetic relations developed in this work are capable of capturing the physical phenomenon only close to the equilibrium. Our aim is to present a rigorous framework for dealing problems of great utility in polycrystalline materials and to demonstrate the efficacy of the proposed set of governing equations using simple bicrystal and tricrystal arrangements, motivated by recent MD simulation studies. Although the tricrystal system is much simpler than the real polycrystal which would consist of numerous grains (generally polyhedral) and triple junctions, we expect the essential features of the model, like drag induced by junctions on GB motion and grain rotation, to remain valid. In any case, extending the present formulation to a real polycrystal with many grains is only a problem of greater computational effort and should be straightforward.

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