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ANALYSIS OF STRESS-DRIVEN GRAIN BOUNDARY DIFFUSION. PART II: DEGENERACY*

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Abstract. The stress-driven grain boundary diffusion problem is a continuum model of mass transport phenomena in microelectronic circuits due to high current densities (electromigration) and gradients in normal stress along grain boundaries. The model involves coupling many different equations and phenomena, and difficulties such as nonlocality, complex geometry, and singularities in the stress tensor have left open such mathematical questions as existence of solutions and compatibility of boundary conditions. In this paper and its companion, we address these issues and establish a firm mathematical foundation for this problem.

We study the properties of a type of Dirichlet-to-Neumann map that involves solving the Lamé equations with interesting interface boundary conditions. We identify a new class of degenerate grain boundary networks that lead to unsuppressed linear growth modes that are suggestive of continental drift in plate tectonics. We use techniques from semigroup theory to prove that the problem is well posed and that the stress field relaxes to a steady state distribution which may or may not completely balance the electromigration force. In the latter (degenerate) case, the displacements continue to grow without bound along stress-free modes.

Key words. grain boundary, diffusion, electromigration, elasticity, semigroups

AMS subject classifications. 35Q72, 47D03, 74F99

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1. Introduction.

Electromigration is a diffusion process in which high current densities act as a driving force to transport ions in a metallic lattice in the direction of electron flow by transferring momentum through scattering [10]. As microelectronic circuits become smaller and current densities become higher, failure due to electromigration damage in interconnect lines becomes an everincreasing problem in the design of circuits. Grain boundaries, void surfaces, and passivation interfaces are fast diffusion paths along which the diffusion constant typically is seven to eight orders of magnitude higher than in the grains; therefore, most of the mass transport occurs at these locations. The inhomogeneous redistribution of atoms leads to the development of stresses in the line. Stress gradients along grain boundaries and surface tension at void surfaces both contribute to the flux of atoms, usually suppressing electromigration and increasing the lifetime of the line.

Many experimental, theoretical, and numerical studies have been done to investigate the role of various combinations of electromigration, stress gradients, surface

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diffusion, temperature, and anisotropy on the transport of atoms in the bulk grains, along void surfaces, along grain boundaries, and at passivation interfaces. We refer the reader to the companion paper [13] for a discussion of this literature.

The goal of this paper and its companion [13] is to provide a rigorous treatment of a modest subset of the mass transport phenomena that occur in microelectronic circuits. In particular, our model is two dimensional and neglects void evolution, curvature-driven grain boundary motion, plastic deformation, and thermal effects. Instead, we focus on the coupling of electromigration to stress generation, which is difficult due to nonlocality, stiffness, complex geometry, and stress singularities at junctions where boundary conditions involving normal stress are imposed.

In [13], we describe the problem physically, state the equations and boundary conditions, find an exact solution for an infinite interconnect line, recast the problem for a finite geometry as an ordinary differential equation on a Hilbert space involving two unbounded operators L and S, analyze the operator L, and prove that the problem is well posed (using techniques from semigroup theory) under the simplifying assumption that the grain boundary network is nondegenerate. We summarize many of these results in section 2.

In section 3, we prove that S (a type of Dirichlet-to-Neumann map) is self-adjoint, negative, closed, and densely defined. These properties are stated (omitting proofs) in [13] and play an essential role in our analysis of the nondegenerate and general cases. To define S, we study weak solutions to the grain boundary normal stress problem. This leads us to identify a new class of degenerate grain boundary networks for which S has a nontrivial (but always finite dimensional) kernel. We use an energy argument to prove self-adjointness and negativity, and we present a counting argument that is useful for characterizing degeneracy.

In section 4, we prove that the equation governing the evolution of normal stress on the grain boundary network Γ generates an analytic semigroup of bounded linear operators on $H^1(\Gamma)$. We also show how to use this semigroup to determine the evolution of displacement and stress inside each grain, which is a nontrivial task since the grain boundary normal stress problem is not uniquely solvable in the degenerate case without additional information about the jump in displacement across Γ. We show that the stress field relaxes to a steady state distribution which may or may not completely balance the electromigration force along grain boundaries. In the latter (degenerate) case, the displacement field describing the motion of the grains continues to grow without bound along stress-free modes, leading to behavior that resembles continental drift in plate tectonics.

We remark that such growth modes are quite harmless to an interconnect line. They correspond to a gradual transport of material from one side of each participating grain to the other, causing it to continually drift to avoid misfit with its neighbors, but not leading to stress generation or voiding.

2. Preliminaries. We model the interconnect line as a union $\Omega = \bigcup_{k=1}^{M} \Omega_k$ of disjoint polygonal grains, as shown in Figure 2.1. We denote the outer boundary (the "walls") of the domain by Γ_0, and we denote the grain boundary network by $\Gamma = \bigcup_{j=1}^{N} \Gamma_j$. Each line segment Γ_j is given an arbitrary orientation (a unit tangent vector $\mathbf{t}_j$) and an arc length parameter s which increases in the $\mathbf{t}_j$ direction. The unit normal $\mathbf{n}_j$ points from right ($-$) to left ($+$) facing along $\mathbf{t}_j$. The net grain growth g is defined on Γ as the jump in normal component of displacement across the grain

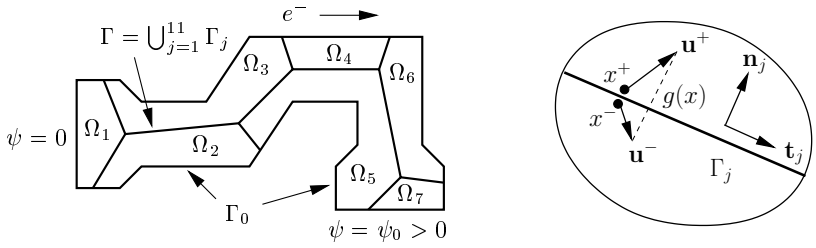

FIG. 2.1. *Left: geometry of an interconnect line. Right: $g(x)$ is the jump in normal component of displacement across Γ at x.*

boundary:

$$g(x) := [\mathbf{u}(x^+) - \mathbf{u}(x^-)] \cdot \mathbf{n}_j \qquad (x \in \Gamma_j). \tag{2.1}$$

It represents the distance the original grains have separated to accommodate the new material that occupies that space; see Figure 2.1. Note that g evolves as a function defined on Γ as $\mathbf{u}$ evolves on Ω; both Γ and Ω remain *fixed* in the reference configuration. The sign of g is independent of the orientation chosen for the segment.

The electric potential ψ is found by solving the Laplace equation subject to the boundary conditions $\psi = 0$ and $\psi = \psi_0$ at the two ends of the interconnect line and $\partial_n \psi = 0$ on all other walls. We assume the grain boundaries do not significantly affect the flow of electrons in the line, so boundary conditions are specified along Γ_0 only; Γ is invisible to ψ.

Each grain is assumed to deform elastically (assuming plane strain) and to satisfy the Lamé equations of linearized elasticity, $\mu \Delta \mathbf{u} + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) = \mathbf{0}$. The outer walls are assumed to be perfectly rigid, giving the two boundary conditions

$$\mathbf{u}(x) = \mathbf{0} \qquad (x \in \Gamma_0). \tag{2.2}$$

Along grain boundaries, four interface boundary conditions are specified:

$$\mathbf{u}(x^+) - \mathbf{u}(x^-) = g(x)\mathbf{n_j} \qquad (x \in \Gamma_j), \tag{2.3}$$

$$\sigma(x^+)\mathbf{n_j} = \sigma(x^-)\mathbf{n_j} \qquad (x \in \Gamma_j). \tag{2.4}$$

In other words, grains are not allowed to slide tangentially, the jump in normal component of displacement is specified to be $g(x)$, and both components of traction balance across the grain boundary. The traction condition is justified because we have adopted an Eulerian viewpoint for the meaning of displacement; see [13]. For a given deformation φ, $\mathbf{u}(x)$ is defined to be $x - \varphi^{-1}(x)$ rather than $\varphi(x) - x$. As a result, $g(x)\mathbf{n}_j = \varphi^{-1}(x^-) - \varphi^{-1}(x^+)$ rather than $\varphi(x^+) - \varphi(x^-)$ (the latter is shown in Figure 2.1). The material and Eulerian viewpoints have the same linearization.

After nondimensionalizing [13], the flux J of atoms along the grain boundary is given by $J = \partial_s(\eta + \psi)$. Here $\eta = \mathbf{n} \cdot \sigma \mathbf{n}$ is the normal stress along the grain boundary, $\psi = \psi\big|_\Gamma$ is the restriction of the electric potential to the grain boundary, and ∂_s is the derivative with respect to arc length along the grain boundary. The continuity equation expressing mass conservation is $\partial_t g + \partial_s J = 0$; hence the evolution of net grain growth is governed by

$$\partial_t g = -\partial_s^2(\eta + \psi) = L(Sg + \psi). \tag{2.5}$$

Here $L = -\frac{\partial^2}{\partial s^2}$ is the negative of the second derivative operator with respect to arc length on each grain boundary segment, and S maps a displacement jump g defined on Γ to the corresponding normal stress η on Γ by solving the Lamé equations, as discussed above. If we apply the operator S to both sides of (2.5), we obtain a differential equation for η:

$$\partial_t \eta = SL(\eta + \psi). \tag{2.6}$$

The solution to this equation is given by $\eta(t) = E_t(\eta + \psi) - \psi$, where $\{E_t : t \geq 0\}$ is the strongly continuous semigroup of linear operators generated by SL; see section 4. The solution to (2.5) is more complicated; it will be discussed in section 4.3.

Boundary conditions for chemical potential continuity and flux balance at junctions are enforced by requiring that $\eta + \psi$ belongs to the domain $\mathcal{D}(L)$ for $t > 0$; see [13]. Similarly, to ensure that g is actually a displacement jump, i.e., that there exists a displacement field $\mathbf{u}$ on Ω satisfying (2.3), we require that $g \in \mathcal{D}(S)$ for $t > 0$.

The domain $\mathcal{D}(S)$ is difficult to characterize; see section 3.3. To describe the domain $\mathcal{D}(L)$, it is useful to establish further notation. Let $C(\Gamma)$ denote the space of continuous functions on Γ, and let $\widetilde{C}(\Gamma)$ denote the space of functions f continuous on the interiors of the Γ_j with well-defined limits $f(x_i^j)$ at the endpoints x_i of Γ_j but with possibly different limiting values at x_i when approached from different segments. Differentiation is defined segment by segment, where we recall that each segment is given an arbitrary orientation along which the arc length parameter increases. We define

$$\widetilde{C}^r(\Gamma) = \{f : f^{(k)} \in \widetilde{C}(\Gamma),\ 0 \leq k \leq r\}. \tag{2.7}$$

Then the domain $\mathcal{D}(L)$ satisfies

$$\{f \in \widetilde{C}^2(\Gamma) : f \text{ satisfies } (*)\} \ \subset\ \mathcal{D}(L)\ \subset\ \{f \in \widetilde{C}^1(\Gamma) : f \text{ satisfies } (*)\}, \tag{2.8}$$

where $(*)$ refers to continuity and flux boundary conditions at all junctions. In other words, $f \in \widetilde{C}^r(\Gamma)$ satisfies $(*)$ if $f \in C(\Gamma)$ and at each junction x_i, $\sum_j \pm f'(x_i^j) = 0$, where the sum is over segments incident to x_i and the sign depends on whether the segment is parameterized toward or away from the junction.

Other key properties of L (all proved in [13]) are as follows. L is self-adjoint and positive. Its kernel consists of the functions

$$e_k(x) = \begin{cases} |\Gamma_{J_k}|^{-\frac{1}{2}}, & x \in \Gamma_{J_k}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.9}$$

Here J_k is the set of indices such that $\Gamma_{J_k} := \cup_{j \in J_k} \Gamma_j$ is the kth connected component of Γ (treated as a point set in $\mathbb{R}^2$), and $|\Gamma_{J_k}| = \sum_{j \in J_k} |\Gamma_j|$ is the sum of the lengths of the segments making up component k. Let $d = \dim \ker(L)$, and define

$$P = I - \sum_{k=1}^{d} (\cdot, e_k) e_k, \quad A = L + \sum_{k=1}^{d} (\cdot, e_k) e_k, \quad G = A^{-1} - \sum_{n=1}^{d} (\cdot, e_k) e_k, \tag{2.10}$$

where $(\cdot, \cdot)$ is the L^2 inner product on Γ. Then P is the orthogonal projection onto the subspace

$$\operatorname{ran}(L) = \ker(L)^{\perp} = \left\{ f \in L^2(\Gamma)\ :\ \int_{\Gamma_{J_k}} f\, ds = 0,\ 1 \leq k \leq d \right\}, \tag{2.11}$$

and we have $L = AP = PA$, $LG = P$, and $GL = P\big|_{\mathcal{D}(L)}$. $A^{\frac{1}{2}}$ is an isomorphism from $H^1(\Gamma)$ to $L^2(\Gamma)$, where $H^1(\Gamma)$ consists of all $f \in C(\Gamma)$ which are absolutely continuous with (weak) derivative $f' \in L^2(\Gamma)$. Finally, $\mathcal{D}(L^{\frac{1}{2}}) = H^1(\Gamma)$.

3. Elasticity with interface boundary conditions. In this section we give rigorous definitions of the operators S and B, define weak solutions to the Lamé equations with appropriate interface boundary conditions along grain boundaries, and introduce the notion of degeneracy of a grain boundary network. We prove that S and B are self-adjoint and negative on $L^2(\Gamma)$, that the former is closed and densely defined, and that the latter is compact. We also provide a precise characterization of grain boundary degeneracy that is easy to check numerically.

In the previous section, we described S as a type of Dirichlet-to-Neumann operator that takes a displacement jump g on the grain boundary, solves the Lamé equations subject to the boundary conditions (2.2)–(2.4), and returns the normal stress η on Γ. For technical reasons, it is preferable to define S as the pseudoinverse of B, where B takes a specified normal stress η on the grain boundary, solves the Lamé equations subject to the boundary conditions

$$\mathbf{u}(x) = \mathbf{0} \qquad (x \in \Gamma_0), \tag{3.1}$$

$$[\mathbf{u}(x^+) - \mathbf{u}(x^-)] \cdot \mathbf{t}_j = 0 \qquad (x \in \Gamma_j), \tag{3.2}$$

$$[\sigma(x^+) - \sigma(x^-)]\mathbf{n}_j = \mathbf{0} \qquad (x \in \Gamma_j), \tag{3.3}$$

$$\mathbf{n}_j \cdot \sigma(x)\mathbf{n}_j = \eta(x) \qquad (x \in \Gamma_j), \tag{3.4}$$

and returns the jump in the normal component of displacement

$$(B\eta)(x) = [\mathbf{u}(x^+) - \mathbf{u}(x^-)] \cdot \mathbf{n}_j \qquad (x \in \Gamma_j). \tag{3.5}$$

The primary obstacle to this approach is that in the case of degeneracy, η must satisfy further conditions for a solution $\mathbf{u}$ to exist, and these solutions are not unique. In this case, we define B using appropriate projections so that its pseudoinverse S has the physical meaning described previously.

3.1. Boundary conditions. To impose Dirichlet boundary conditions at walls and no-slip boundary conditions across grain boundaries, we employ a Hilbert subspace H of $H^1(\Omega)^2$ defined as the kernel of appropriate trace operators. Recall that the inner product of the Sobolev space $H^1(\Omega)^2$ is given by

$$(\mathbf{u}, \mathbf{v}) = \int_\Omega (\mathbf{u} \cdot \mathbf{v} + \nabla \mathbf{u} : \nabla \mathbf{v}) dx, \tag{3.6}$$

where $(\nabla \mathbf{u})_{ij} = \partial_j u_i$ and $A : B = \sum_{ij} A_{ij} B_{ij}$. Note that the values of $\mathbf{u}$ in this space do not communicate across grain boundaries—the restriction of $\mathbf{u}$ to each Ω_k can be any function in $H^1(\Omega_k)^2$. The trace operators defined below map, respectively, a vector field $\mathbf{u} \in H^1(\Omega)^2$ to its value at the walls, to its jump in tangential component across grain boundaries, and to its jump in normal component across grain boundaries. We use γ_0 and γ_t to define the Hilbert space H given by

$$H = \left\{ \mathbf{u} \in H^1(\Omega)^2 \;\middle|\; \gamma_0 \mathbf{u} = \mathbf{0},\ \gamma_t \mathbf{u} = 0 \right\}. \tag{3.7}$$

We will need γ_n in section 3.3 to define weak solutions and also to define the operator B. Recall that N and M are the number of grain boundary segments and the

number of regions, respectively:

$$\Omega = \bigcup_{k=1}^{M} \Omega_k, \qquad \Gamma = \bigcup_{j=1}^{N} \Gamma_j, \qquad \Gamma_0 = \text{outer walls.} \tag{3.8}$$

THEOREM 3.1. *The following trace operators are compact:*

$$\gamma_0 : H^1(\Omega)^2 \to L^2(\Gamma_0)^2 : \mathbf{u} \mapsto \mathbf{u}\big|_{\Gamma_0}, \tag{3.9}$$

$$\gamma_t : H^1(\Omega)^2 \to L^2(\Gamma) : \mathbf{u} \mapsto \left([\mathbf{u}\big|_{\Gamma_1^+} - \mathbf{u}\big|_{\Gamma_1^-}] \cdot \mathbf{t}_1 \, , \, \ldots \, , \, [\mathbf{u}\big|_{\Gamma_N^+} - \mathbf{u}\big|_{\Gamma_N^-}] \cdot \mathbf{t}_N \right), \tag{3.10}$$

$$\gamma_n : H^1(\Omega)^2 \to L^2(\Gamma) : \mathbf{u} \mapsto \left([\mathbf{u}\big|_{\Gamma_1^+} - \mathbf{u}\big|_{\Gamma_1^-}] \cdot \mathbf{n}_1 \, , \, \ldots \, , \, [\mathbf{u}\big|_{\Gamma_N^+} - \mathbf{u}\big|_{\Gamma_N^-}] \cdot \mathbf{n}_N \right). \tag{3.11}$$

Here $\mathbf{u}\big|_{\Gamma_j^+}$ *is the trace of* $\mathbf{u}$ *on* Γ_j *from the left (i.e., the trace of* $\mathbf{u}\big|_{\Omega_k}$ *on* Γ_j*, where* Ω_k *lies to the left of* Γ_j*),* $\mathbf{u}\big|_{\Gamma_j^-}$ *is the trace of* $\mathbf{u}$ *on* Γ_j *from the right, and we have identified* $L^2(\Gamma)$ *with* $L^2(\Gamma_1) \times \cdots \times L^2(\Gamma_N)$.

Proof. Since Γ_0 is also a union of line segments, it suffices to show that for any region Ω_k and boundary segment $X \subset \partial\Omega_k$, the composite map

$$\mathbf{u} \mapsto \mathbf{u}\big|_{\Omega_k} \mapsto \left(\mathbf{u}\big|_{\Omega_k}\right)\big|_{\partial\Omega_k} \mapsto \left(\mathbf{u}\big|_{\Omega_k}\right)\big|_X \tag{3.12}$$

is compact. The first and last maps are just restriction operators from $H^1(\Omega)^2$ to $H^1(\Omega_k)^2$ and $L^2(\partial\Omega_k)^2$ to $L^2(X)^2$, so they are bounded. Since Ω_k is a polygon, it has a Lipschitz boundary, and hence [1, 4, 5] the trace operator

$$\gamma_k : H^1(\Omega_k)^2 \to H^{\frac{1}{2}}(\partial\Omega_k)^2 \tag{3.13}$$

is bounded. But $H^{\frac{1}{2}}(\partial\Omega_k)^2$ is compactly embedded in $L^2(\partial\Omega_k)^2$, so the middle map in (3.12) is compact, as required. ∎

3.2. Degenerate grain boundary networks. In this section we define the notion of grain boundary degeneracy, which characterizes the existence of unsuppressed growth modes consisting of stress-free infinitesimal rigid body motions in each grain. We also describe an algorithm for determining whether a given grain boundary network is degenerate and, if it is, for finding these modes. We present a counting argument that strongly suggests that grain geometries with convex grains and very few quadruple or higher order junctions will be nondegenerate. We verify numerically that randomly generated grain boundary networks with convex grains are indeed nondegenerate.

DEFINITION 3.2. *A grain boundary network* Γ *is said to be* degenerate *if* H *contains a nonzero function* $\mathbf{u}$ *consisting of infinitesimal rigid body motions (defined below) on each grain.*

To gain geometric insight, we construct a procedure for testing the degeneracy of a given grain boundary network. An infinitesimal rigid body motion is a displacement field of the form

$$u_1(x, y) = a - cy, \qquad u_2(x, y) = b + cx, \tag{3.14}$$

where a, b, c are arbitrary real numbers. Let (x_k, y_k) be some fixed point in Ω_k, and let r_k be a characteristic length scale for the kth grain. For any $\mathbf{u} \in H(\Omega)^2$ consisting

of infinitesimal rigid body motions, there are parameters a_k, b_k, and c_k for each region such that

$$\mathbf{u}\big|_{\Omega_k} = \left(a_k - c_k \frac{y - y_k}{r_k},\, b_k + c_k \frac{x - x_k}{r_k}\right). \tag{3.15}$$

We wish to determine if there is a nontrivial choice of these parameters such that the corresponding $\mathbf{u}$ belongs to H. We define the vector w by

$$w = (a_1, b_1, c_1, \ldots, a_M, b_M, c_M)^T \tag{3.16}$$

and construct a matrix A with $3M$ columns such that

$$Aw = 0 \;\Leftrightarrow\; \mathbf{u}_w \in H. \tag{3.17}$$

Clearly, if Ω_k touches an outer wall, then the condition that $\gamma_0 \mathbf{u} = 0$ requires that $a_k = b_k = c_k = 0$. We assume that the M_0 outer grains appear first in the list, and we let

$$A_{ij} = \delta_{ij} \qquad (1 \le i \le 3M_0,\, 1 \le j \le 3M) \tag{3.18}$$

so that A has the block structure

$$A = \begin{pmatrix} I & 0 \\ * & A' \end{pmatrix}. \tag{3.19}$$

Note that A is injective iff A' is injective. For each edge that borders a grain with index $k > M_0$, we add a row to A to impose the condition that $\gamma_t \mathbf{u} = 0$. Explicitly, letting (x, y) be any point on edge j and denoting the left and right grains by l and k, the row added to A enforces the equation

$$\left(a_l - c_l \frac{y - y_l}{r_l} - a_k + c_k \frac{y - y_k}{r_k},\, b_l + c_l \frac{x - x_l}{r_l} - b_k - c_k \frac{x - x_k}{r_k}\right) \cdot \mathbf{t}_j \;=\; 0, \tag{3.20}$$

which is clearly linear in the components of w. Note that adding $\alpha \mathbf{t}_j$ to (x, y) does not affect the validity of this equation, so if it holds for one point on the edge, it holds at all points on the edge.

The number of edges that contribute an equation to A can be computed as follows. Let $\Omega' = \cup_{k=M_0+1}^{M} \Omega_k$, and consider the planar graph $\Gamma' = \partial\Omega'$. For example, in Figure 3.1(a), Γ' consists of the eight segments bordering unshaded regions. The Euler relation

$$n + f - e = 1 \qquad (\Gamma' \text{ connected}) \tag{3.21}$$

gives the relationship between the number of vertices, regions, and edges of this graph, where we use 1 instead of 2 since we do not count the unbounded region. If $\overline{\Omega'}$ is multiply connected, this formula holds for each of the c connected subgraphs of Γ', so (3.21) should be modified to read

$$n + f - e = c \qquad (\Gamma' \text{ has } c \text{ connected components}). \tag{3.22}$$

Let n_p be the number of vertices with p incident edges. Then since each edge has two endpoints, we have

$$\sum_{p=2}^{\infty} p n_p = 2e. \tag{3.23}$$

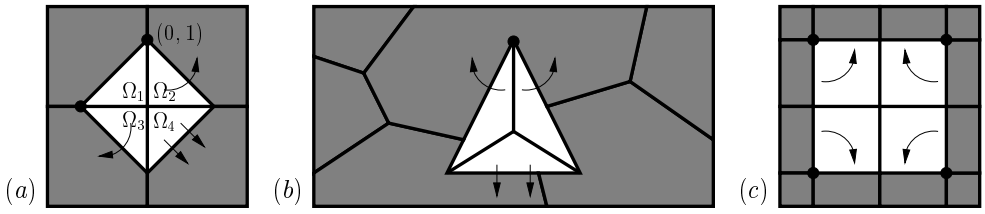

FIG. 3.1. *Examples of degenerate grain boundary networks.* (a) Ω' *has four regions and eight edges, so* A' *has* $12-8=4$ *more columns than rows. This also could have been obtained using* (3.24) *with* $n_3=4, n_4=1$. *The arrows represent one of the functions* $\mathbf{u}$ *in the four dimensional space* H_d, *namely,* $\mathbf{u}\big|_{shaded}=\mathbf{u}\big|_{\Omega_1}=\mathbf{0}$, $\mathbf{u}\big|_{\Omega_2}=(1-y,x)$, $\mathbf{u}\big|_{\Omega_3}=(y,-1-x)$, $\mathbf{u}\big|_{\Omega_4}=(1,-1)$. (b) A' *has six rows and nine columns. Note that nonconvexity in the outer grains allows all nodes of* Ω' *to have* $p=3$, *whereas normally* $n_2\geq 3$. (c) *This time* A' *has the same number of rows and columns, yet it still has a one dimensional kernel since the sign pattern* $+-+-$ *is periodic at a quadruple junction.*

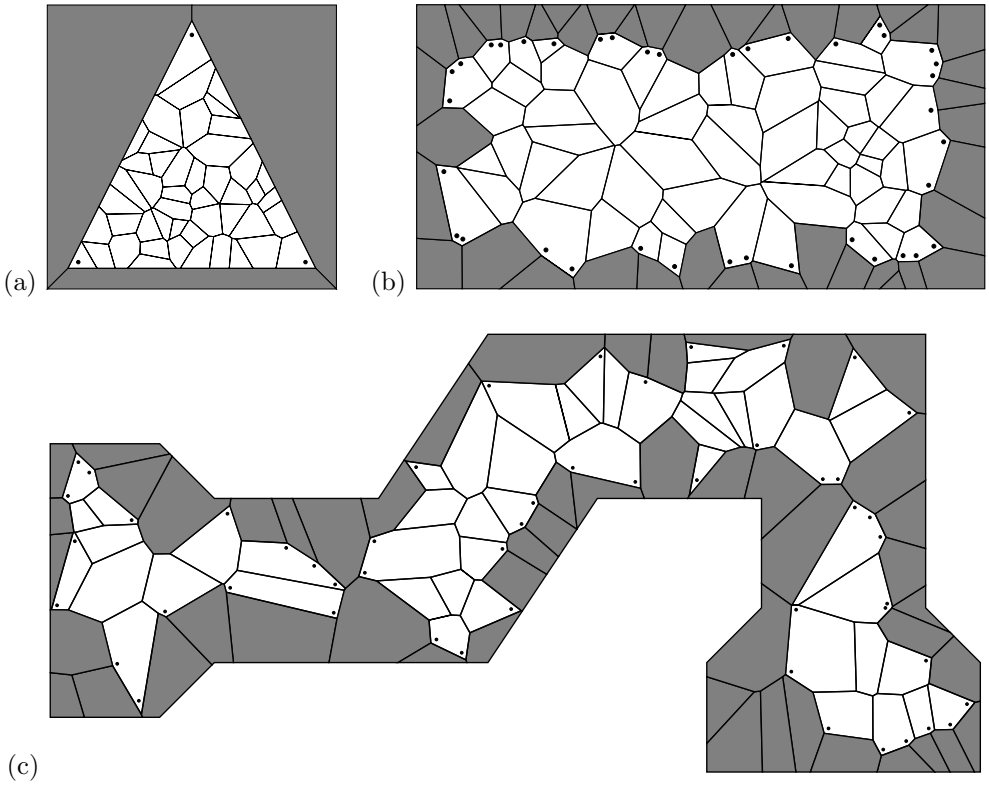

FIG. 3.2. *Typical examples of the geometries generated while computing the condition numbers in Table* 3.1. *Each* • *marks a corner with* $p=2$ *incident edges. All other junctions of* Γ' *have* $p=3$. *Triple junctions often occur clustered together in random Voronoi diagrams, giving the appearance of higher order junctions; this does not give rise to poorly conditioned matrices* A'. *Large shear forces may develop across short edges in such cases if there is not enough redundancy in the other equations (e.g., in case* (a) *here), but that is not a relevant issue when deciding whether a grain boundary network is degenerate. Since at least three corners with* $p=2$ *are needed to traverse the outer boundary of each connected component of* Γ', $e-3f$ *in* (3.24) *is guaranteed to be nonnegative.* (a) *Same number of equations as unknowns* ($e=3f$). (b) $n_2=38$, *so there are* $n_2-3=35$ *more equations than unknowns.* (c) $n_2=51$ *and* $c=3$, *so* $e-3f=42$. *Nonconvexity of grains at outer walls due to reentrant corners clearly will not lead to the difficulties that arose in Figure* 3.1(b).

TABLE 3.1

Condition number of A' for randomly generated Voronoi diagrams. The geometry labels correspond to Figure 3.2*, which shows examples of* (a)-50, (b)-100, *and* (c)-100. *In case* (a)*, we add three outer regions to the Voronoi diagram so that the number of equations is equal to the number of unknowns (a worst-case scenario). Geometries* (b) *and* (c) *are more realistic, although they tend to have more pathologies (such as clustered triple points and short edges) than would likely be found in a real grain boundary network. All the matrices tested were extremely well conditioned, which supports our conjecture that if each grain is convex and no quadruple or higher order junctions occur in the grain boundary network, then Γ is nondegenerate.*

Geometry	Regions	Trials	max	min	mean	std dev
(a)	200	10000	172.6	31.7	37.8	3.2
(a)	100	10000	48.4	21.6	26.2	2.1
(a)	50	10000	35.0	14.4	18.2	1.6
(b)	200	10000	31.8	13.0	16.8	1.3
(b)	100	10000	31.5	8.2	11.1	1.1
(c)	200	10000	26.8	7.4	9.9	1.1
(c)	100	10000	21.4	4.5	6.9	1.1

Multiplying (3.22) by 3 and subtracting (3.23), we obtain

$$e - 3f = \sum (3-p)n_p - 3c \qquad (A' \text{ is an } e \times 3f \text{ matrix}). \tag{3.24}$$

Since each region of Ω' contributes three unknowns and each edge contributes one equation, we see that a necessary condition for the grain boundary network to be nondegenerate is that the right-hand side be nonnegative—otherwise A' will have more columns than rows, and hence a nontrivial kernel. This necessary condition is automatically satisfied if each grain is convex and $n_p = 0$ for $p > 3$, i.e., if we require that all grain boundary junctions be gb-wall or triple junctions: traversing the outer boundary of each of the c components of $\overline{\Omega'}$, we will encounter at least three changes in direction of more than 180 degrees; each of these angles contributes to n_2 since the third segment must prevent nonconvex outer grains (the grains touching walls), and thus $n_2 \geq 3c$. Some examples of degenerate grain boundary networks are shown in Figure 3.1.

CONJECTURE 3.3. *If each Ω_k is convex and no quadruple or higher order junctions occur in the grain boundary network, then Γ is nondegenerate.*

To test this conjecture, we wrote a PERL program to choose M points at random in a polygonal domain U, compute the Voronoi diagram of these points, chop Voronoi regions that cross ∂U, set up the matrix A', and call Matlab to compute its condition number as the ratio of largest to smallest singular value. The points (x_k, y_k) are taken to be the average of the vertices of grain k, and r_k is taken to be $\sqrt{\text{area}_k/\pi}$. The purpose of x_k, y_k, and r_k is to improve the condition number of A' by scaling the effect of c_k to be commensurate with a_k and b_k. The PERL program repeats the above procedure many times (opening a pipe to Matlab at the beginning) and computes the minimum, maximum, mean, and standard deviation of the condition numbers. The results are summarized in Table 3.1. Typical examples of the resulting grain boundary structures are shown in Figure 3.2. Although convex grains do not necessarily arise from Voronoi diagrams, we see no reason that these would not be a good representative sample, especially in light of the fact that *all* the matrices A' that we generated in this way were extremely well conditioned even for grain boundary networks where several triple points had almost coalesced into higher order junctions.

Even if the conjecture is false, this numerical experiment shows that "typical" grain boundary networks are nondegenerate, and we have provided a method for

finding all degeneracies of any grain boundary network (possibly containing nonconvex grains and higher order junctions):

PROCEDURE 3.4 (finding all degeneracies). *Construct the matrix A, find a basis $w_1, \dots, w_q$ for its kernel, and record the corresponding displacements $\mathbf{u}_1, \dots, \mathbf{u}_q$ using* (3.15) *and* (3.16). *These are a basis for the subspace H_d of stress-free (grain by grain) infinitesimal rigid body motions in H.*

DEFINITION 3.5. *A* degenerate grain growth mode *is a function $h \in L^2(\Gamma)$ of the form $h = \gamma_n(\mathbf{u})$ for some $\mathbf{u} \in H_d$. We denote the space of such functions by $\gamma_n(H_d)$.*

Remark 3.6. We will see later that $\ker(S) = \ker(B) = \gamma_n(H_d)$.

LEMMA 3.7. *γ_n is injective on H_d. Thus if $\{\mathbf{u}_k\}_{k=1}^q$ is a basis for H_d, then the functions $h_k = \gamma_n(\mathbf{u}_k)$ form a basis for $\gamma_n(H_d)$.*

Proof. Suppose $\mathbf{u} \in H_d$ and $\gamma_n(\mathbf{u}) = 0$. Then, since $H_d \subset H$, we also have $\gamma_t(\mathbf{u}) = 0$ and $\gamma_0(\mathbf{u}) = 0$. Thus $\mathbf{u}$ is continuous across grain boundaries, is zero on the outer walls, and consists of infinitesimal rigid body motions on each grain. Continuity across grain boundaries implies that the rigid body parameters are the same in each grain, for if l and r index the parameters on either side of a grain boundary segment, then

$$\begin{aligned} a_l - a_r - (c_l - c_r)y &= 0, \\ b_l - b_r + (c_l - c_r)x &= 0 \end{aligned} \tag{3.25}$$

for each (x, y) on the segment. Using two points on the grain boundary, we find $c_l = c_r$, so (3.25) implies $a_l = a_r$ and $b_l = b_r$. Dirichlet conditions at the walls then give that $a = b = c = 0$ in all grains, as required. ∎

Remark 3.8. We may assume the h_k are orthonormal in $L^2(\Gamma)$ (using a Gram–Schmidt procedure, if necessary).

THEOREM 3.9. *Each $h \in \gamma_n(H_d)$ has zero mass on every connected component of the grain boundary network:*

$$\int_{\Gamma_{J_i}} h \, ds = 0 \qquad (i = 1, \dots, d). \tag{3.26}$$

Proof. Let $\mathbf{u} \in H_d$, $h = \gamma_n \mathbf{u}$, and $i \in \{1, \dots, d\}$. Define

$$K_i = \{k : \Omega_k \text{ does not touch } \Gamma_0 \text{ but does touch } \Gamma_{J_i}\}, \tag{3.27}$$

$$J_i' = \{j \in J_i : \Gamma_j \text{ borders an } \Omega_k \text{ which doesn't touch } \Gamma_0\}. \tag{3.28}$$

In Figure 3.3, J_1' contains 12 segment indices, K_1 contains 4 region indices, J_2' contains 6 indices, K_2 contains 3 indices, and J_3' and K_3 are empty. Since $\mathbf{u}$ is an infinitesimal rigid body motion on each grain, it is divergence free, so for $1 \le k \le M$ we have

$$\int_{\partial\Omega_k} \mathbf{u} \cdot \mathbf{n} \, ds = \iint_{\Omega_k} \nabla \cdot \mathbf{u} \, dx = 0 \qquad (\mathbf{n} = \text{outward unit normal}). \tag{3.29}$$

Summing (3.29) over $k \in K_i$ (with an empty sum meaning zero), we obtain

$$0 = \sum_{k \in K_i} \int_{\partial\Omega_k} \mathbf{u} \cdot \mathbf{n} \, ds = \sum_{j \in J_i'} \int_{\Gamma_j} [\mathbf{u}(x^-) - \mathbf{u}(x^+)] \cdot \mathbf{n}_j \, ds = \int_{\Gamma_{J_i}} -h \, ds. \tag{3.30}$$

Here we have used the following facts: $\mathbf{n}_j$ is the unit inward normal on the left $(+)$ grain and the unit outward normal on the right $(-)$ grain; the condition $\gamma_0 \mathbf{u} = \mathbf{0}$

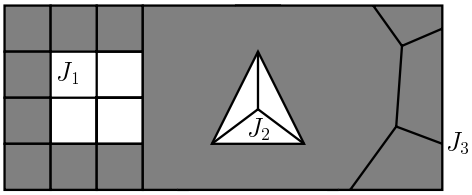

FIG. 3.3. *Shown here, Γ consists of three connected components Γ_{J_i}, so $\dim\ker(L) = 3$. The space H_d (and hence $\ker(S)$) is four dimensional (one degree of freedom in the unshaded structure on the left, three in the middle; see Figure* 3.1*). Each $\mathbf{u} \in H_d$ is zero on the shaded grains.*

implies that $\mathbf{u}$ is zero on any Ω_k touching an outer wall since $\mathbf{u}$ consists of infinitesimal rigid body motions; if $j \in J_i'$, then Γ_j borders either one or two Ω_k with $k \in K_i$—in the former case, $\mathbf{u}(x^{\pm})$ is zero on the other side because that region touches a wall; if $k \in K_i$, all boundary segments Γ_j of Ω_k have $j \in J_i'$; finally, $h = \gamma_n \mathbf{u}$ is zero on the segments Γ_j with $j \in J_i \setminus J_i'$ since both adjacent regions touch a wall. Figure 3.4 illustrates a similar argument in the next section. ∎

3.3. Weak solutions. In this section, we define weak solutions of the grain boundary normal stress and displacement jump problems, and we give rigorous definitions of the operators B and S. Many complications arise in the case of degenerate grain boundaries that make the analysis difficult. We prove that B is compact, self-adjoint, and negative, and we show that $\ker(B) = \gamma_n(H_d)$. The operator S is defined as the pseudoinverse of B, inheriting self-adjointness and negativity.

We will need to make use of the bilinear form

$$a(\mathbf{u}, \mathbf{v}) := \int_\Omega \sigma(\mathbf{u}) : \varepsilon(\mathbf{v})\, dx = \int_\Omega [\lambda\, (\nabla \cdot \mathbf{u})(\nabla \cdot \mathbf{v}) + 2\mu\, \varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v})]\, dx, \tag{3.31}$$

which induces the seminorm $\|\mathbf{u}\|_a = \sqrt{a(\mathbf{u}, \mathbf{u})}$ on $H^1(\Omega)^2$. Here

$$\varepsilon(\mathbf{u})_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i), \qquad \sigma(\mathbf{u}) = \lambda \operatorname{tr} \varepsilon(\mathbf{u}) I + 2\mu\varepsilon(\mathbf{u}), \tag{3.32}$$

and there is clearly a constant C such that

$$\|\mathbf{u}\|_a \le C\|\mathbf{u}\|_{H^1(\Omega)^2} \qquad \left(\mathbf{u} \in H^1(\Omega)^2\right). \tag{3.33}$$

For any $\eta \in L^2(\Gamma)$, we define the linear functional $l_\eta \in H'$ by

$$l_\eta(\mathbf{v}) = -(\eta, \gamma_n \mathbf{v})_{L^2(\Gamma)} = -\int_\Gamma (\eta)(\gamma_n \mathbf{v})\, ds \qquad (\mathbf{v} \in H). \tag{3.34}$$

Note that

$$\|l_\eta\|_{H'} \le \|\gamma_n\|_{\mathcal{L}(H^1(\Omega)^2, L^2(\Gamma))} \|\eta\|_{L^2(\Gamma)}. \tag{3.35}$$

DEFINITION 3.10. *A weak solution to the grain boundary normal stress problem for a given normal stress $\eta \in L^2(\Gamma)$ is a function $\mathbf{u} \in H$ which satisfies*

$$a(\mathbf{u}, \mathbf{v}) = -\int_\Gamma (\eta)(\gamma_n \mathbf{v})\, ds \qquad (\mathbf{v} \in H). \tag{3.36}$$

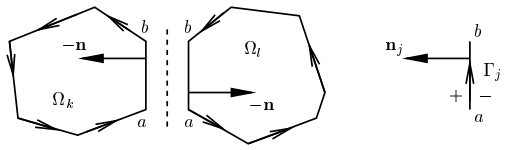

FIG. 3.4. *The contribution of a particular grain boundary segment to* $\sum_k \int_{\partial\Omega_k} \mathbf{v}\big|_{\Omega_k} \cdot \sigma\mathbf{n}$ *contains precisely one term from the left grain and one term from the right grain. Segments on the outer walls do not contribute since* $\gamma_0\mathbf{v} = 0$.

PROPOSITION 3.11. *Any classical solution is a weak solution.*

Proof. Suppose $\mathbf{u}$ is a classical solution with corresponding stress tensor σ and $\mathbf{v} \in H$. Then on Ω_k we have

$$\begin{aligned}(3.37)\qquad \int_{\partial\Omega_k} \mathbf{v}\big|_{\Omega_k} \cdot (\sigma\mathbf{n})\, ds &= \int_{\Omega_k} \partial_j\,(v_i\sigma_{ij})\, dx = \int_{\Omega_k} \overbrace{(\partial_j\sigma_{ij})}^{0}\, v_i + \sigma_{ij}\,(\partial_j v_i)\, dx \\ &= \int_{\Omega_k} \sigma_{ij}\left(\frac{\partial_j v_i + \partial_i v_j}{2}\right) dx = \int_{\Omega_k} \sigma : \varepsilon(\mathbf{v})\, dx = a_k(\mathbf{u}\big|_{\Omega_k},\, \mathbf{v}\big|_{\Omega_k}).\end{aligned}$$

When we sum over all regions, the right-hand side becomes $a(\mathbf{u}, \mathbf{v})$, and the left-hand side becomes a sum over all segments of Γ with one term coming from the left grain and one term coming from the right grain; see Figure 3.4. Since $\gamma_t\mathbf{v} = 0$ and σ is continuous across each segment, the sum of these two terms for the jth segment is

$$(3.38)\qquad \int_{\Gamma_j} (\mathbf{v}^+ \cdot \sigma(-\mathbf{n}_j))\, ds + \int_{\Gamma_j} (\mathbf{v}^- \cdot \sigma\mathbf{n}_j)\, ds = -\int_{\Gamma_j} (\gamma_n\mathbf{v})\mathbf{n}_j \cdot \sigma\mathbf{n}_j\, ds.$$

Summing over all segments and using the boundary condition $\sigma_{nn} = \eta$, we obtain (3.36) as desired. ∎

PROPOSITION 3.12. *If the grain boundary network is degenerate, then a necessary condition for a weak solution to exist is that* $\eta \perp \gamma_n(H_d)$. *If a solution does exist, it is only defined modulo* H_d.

Proof. Fix η, and suppose a solution $\mathbf{u}$ exists. For any $\mathbf{w} \in H_d$, we use (3.36) to conclude that

$$(3.39)\qquad -\int_\Gamma (\eta)(\gamma_n\mathbf{w})\, ds = a(\mathbf{u}, \mathbf{w}) = \int_\Omega \sigma(\mathbf{u}) : \overbrace{\varepsilon(\mathbf{w})}^{0}\, dx = 0.$$

Thus η is orthogonal to $\gamma_n\mathbf{w}$. For any $\mathbf{v} \in H$ we have $a(\mathbf{w}, \mathbf{v}) = 0$, so

$$(3.40)\qquad a(\mathbf{u} + \mathbf{w}, \mathbf{v}) = a(\mathbf{u}, \mathbf{v}) = -\int_\Gamma (\eta)(\gamma_n\mathbf{v})\, ds,$$

and $\mathbf{u} + \mathbf{w}$ is also a weak solution. ∎

DEFINITION 3.13. *We define the space* $\tilde{H}$ *by the relation* $\gamma_n(\tilde{H}) \subset \gamma_n(H_d)^\perp$:

$$(3.41)\qquad \tilde{H} = \{\mathbf{u} \in H \;\big|\; l_h(\mathbf{u}) = 0 \text{ whenever } h \in \gamma_n(H_d)\}.$$

Remark 3.14. Since γ_n is injective on H_d, $\mathbf{u} \equiv 0$ is the only (grain by grain) infinitesimal rigid body motion in $\tilde{H}$, i.e., $\tilde{H} \cap H_d = \{0\}$. Since the codimension of $\tilde{H}$ is at most $q := \dim H_d$ by (3.41), the decomposition $H = \tilde{H} \oplus H_d$ holds.

THEOREM 3.15. *The bilinear form $a(\cdot,\cdot)$ is coercive on $\tilde{H}$, and therefore $\|\cdot\|_a$ is a norm on $\tilde{H}$ equivalent to the one inherited from $H^1(\Omega)^2$.*

Proof. Since $\lambda \geq 0$ and $\mu > 0$, it suffices to show that there is a $c > 0$ such that

$$\|\mathbf{u}\|_\varepsilon^2 := \int_\Omega \varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u})\, dx \geq c \int_\Omega [\mathbf{u}\cdot\mathbf{u} + \nabla\mathbf{u} : \nabla\mathbf{u}]\, dx = c\|\mathbf{u}\|_{\tilde{H}}^2 \qquad \left(\mathbf{u} \in \tilde{H}\right). \tag{3.42}$$

Suppose not. Then there is a sequence of unit vectors $\mathbf{u}_n \in \tilde{H}$ such that

$$\|\mathbf{u}_n\|_\varepsilon^2 \to 0. \tag{3.43}$$

Since the unit ball of $H^1(\Omega)^2$ is compact in $L^2(\Omega)^2$, there is a subsequence which converges in $L^2(\Omega)^2$. Replacing the original sequence with the subsequence, we may assume

$$\|\mathbf{u}_m - \mathbf{u}_n\|_{L^2(\Omega)^2}^2 \to 0 \qquad (m, n \to \infty). \tag{3.44}$$

Since each Ω_k is polygonal, Korn's inequality [4, 3] guarantees the existence of positive constants c_k such that

$$\int_{\Omega_k} \varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u})\, dx + \|\mathbf{u}\|_{L^2(\Omega_k)^2}^2 \geq c_k \|\mathbf{u}\|_{H^1(\Omega_k)^2}^2 \qquad \left(\mathbf{u} \in H^1(\Omega_k)^2\right). \tag{3.45}$$

Letting $c = \min_k c_k$ and summing over all regions, we obtain

$$\|\mathbf{u}\|_\varepsilon^2 + \|\mathbf{u}\|_{L^2(\Omega)^2}^2 \geq c\|\mathbf{u}\|_{H^1(\Omega)^2}^2 \qquad \left(\mathbf{u} \in H^1(\Omega)^2\right). \tag{3.46}$$

Replacing $\mathbf{u}$ by $\mathbf{u}_m - \mathbf{u}_n$ in (3.46) and using (3.43) and (3.44), we find that $\{\mathbf{u}_n\}$ is a Cauchy sequence in $\tilde{H}$. We let $\mathbf{u}^* = \lim_n \mathbf{u}_n$ and note that because $\|\cdot\|_\varepsilon$ is continuous in $H^1(\Omega)^2$, $\|\mathbf{u}^*\|_\varepsilon = \lim_n \|\mathbf{u}_n\|_\varepsilon = 0$. Thus $\varepsilon(\mathbf{u}^*) \equiv 0$. It is straightforward to show [3] that the only solutions to $\varepsilon(\mathbf{u}) \equiv 0$ on a domain U are infinitesimal rigid body motions. Thus $\mathbf{u}^*\big|_{\Omega_k}$ is an infinitesimal rigid body motion for each k, and by Remark 3.14, $\mathbf{u}^* \equiv \mathbf{0}$. But this is impossible since we must also have $\|\mathbf{u}^*\|_{\tilde{H}} = \lim_n \|\mathbf{u}_n\|_{\tilde{H}} = 1$. Therefore $a(\cdot,\cdot)$ is coercive on $\tilde{H}$ as claimed. ∎

PROPOSITION 3.16. *If $\eta \in L^2(\Gamma)$ is nonzero, then $l_\eta \in H'$ is nonzero.*

Proof. We define

$$\mathcal{C} = \{\eta \in \widetilde{C}^1(\Gamma) \cap C(\Gamma) \;\big|\; \eta = 0 \text{ at all junctions}\}, \tag{3.47}$$

where $\widetilde{C}^r(\Gamma)$ was defined in (2.7), and we claim that

$$\mathcal{C} \subset \{\eta \in L^2(\Gamma) \;\big|\; \exists\, \mathbf{v} \in H \text{ s.t. } \eta = \gamma_n \mathbf{v}\}. \tag{3.48}$$

To see this, let $\eta \in \mathcal{C}$, and extend η to $C(\Gamma \cup \Gamma_0)$ by setting $\eta = 0$ on the outer walls. Decompose η into a sum

$$\eta = \sum_k \eta_k, \qquad \eta_k = \frac{1}{2}\eta\big|_{\partial\Omega_k}. \tag{3.49}$$

Since each restriction η_k is C^1 on the (closed) segments of $\partial\Omega_k$ and zero at the corners, the x- and y-components ξ_k^1, ξ_k^2 of $-\eta_k\mathbf{n}$ also have this property ($\mathbf{n}$ is the outward unit normal). This is sufficient to ensure that each ξ_k^i belongs to $H^1(\partial\Omega_k) \subset H^{\frac{1}{2}}(\partial\Omega_k)$, which implies [5] that there are functions $v_k^i \in H^1(\Omega_k)$ whose trace is equal to ξ_k^i

on the boundary. Defining $\mathbf{v} \in H$ grain by grain to have components v_k^1, v_k^2 proves (3.48). Since $\mathcal{C}$ is dense in $L^2(\Gamma)$ and (3.48) holds, we have

$$l_\eta = 0 \quad \Rightarrow \quad \eta \perp \mathcal{C} \quad \Rightarrow \quad \eta = 0 \quad \text{a.e.} \tag{3.50}$$

as desired. ∎

COROLLARY 3.17. *If $\eta \in \gamma_n(H_d)^\perp$ is nonzero, then l_η is nonzero in $\tilde{H}'$.*

Proof. Such an l_η is nonzero when acting on H and is zero on H_d, so it must be nonzero on $\tilde{H}$ due to $H = \tilde{H} \oplus H_d$. ∎

DEFINITION 3.18. *The projection R is defined as the orthogonal projection in $L^2(\Gamma)$ onto $\gamma_n(H_d)^\perp$. Explicitly, we have*

$$R = I - \sum_{k=1}^{q} (\cdot, h_k) h_k, \tag{3.51}$$

where the h_k form an L^2-orthonormal basis for $\gamma_n(H_d)$, as discussed in Remark 3.8.

THEOREM 3.19 (weak solutions). *For any $\eta \in L^2(\Gamma)$, there exists a unique weak solution $\mathbf{u}[\eta] \in \tilde{H}$ to the grain boundary normal stress problem with normal stress $R\eta$ on Γ. There is a constant C independent of η such that*

$$\|\mathbf{u}[\eta]\|_{H^1(\Omega)^2} \leq C \|\eta\|_{L^2(\Gamma)}. \tag{3.52}$$

Moreover, if $\mathbf{u} \equiv 0$, then $\eta \in \gamma_n(H_d)$.

Proof. We produce a candidate solution $\mathbf{u} \in \tilde{H}$ using the Lax–Milgram theorem and the fact that $a(\cdot, \cdot)$ is bounded and coercive on $\tilde{H}$ while $l_{R\eta}$ is a bounded linear functional on $\tilde{H}$. The solution $\mathbf{u}$ is the unique function in $\tilde{H}$ satisfying

$$a(\mathbf{u}, \mathbf{v}) = l_{R\eta}(\mathbf{v}) \qquad (\mathbf{v} \in \tilde{H}), \tag{3.53}$$

which we must show holds for all $\mathbf{v} \in H$. Since $H = \tilde{H} \oplus H_d$, it suffices to check the result for $\mathbf{v} \in H_d$: we have $a(\mathbf{u}, \mathbf{v}) = 0$ since $\mathbf{v}$ is a rigid body motion on each grain, and $l_{R\eta}(\mathbf{v}) = -(R\eta, \gamma_n \mathbf{v}) = 0$ since R projects onto $\gamma_n(H_d)^\perp$. Equation (3.52) follows from coercivity, (3.53), and (3.35):

$$c\|\mathbf{u}\|^2 \leq a(\mathbf{u}, \mathbf{u}) \leq \|l_{R\eta}\| \, \|\mathbf{u}\| \leq \|\gamma_n\| \, \|R\| \, \|\mathbf{u}\| \, \|\eta\|. \tag{3.54}$$

If $\eta \notin \gamma_n(H_d)$, then $R\eta$ satisfies the hypothesis of Corollary 3.17, so $l_{R\eta}$ is nonzero in $\tilde{H}'$. By (3.53), the solution $\mathbf{u}$ cannot be identically zero. ∎

DEFINITION 3.20. *The operator $B : L^2(\Gamma) \to L^2(\Gamma)$ is defined via*

$$B\eta := \gamma_n \mathbf{u}[\eta]. \tag{3.55}$$

Note that in the case of grain boundary degeneracy, $\mathbf{u}[\eta]$ involves a projection of η and a selection criterion for choosing among the nonunique solutions in H.

THEOREM 3.21. *B is compact, self-adjoint, and negative and satisfies*

$$\ker(B) = \gamma_n(H_d). \tag{3.56}$$

Proof. B is compact because $\eta \mapsto \mathbf{u}[\eta]$ is bounded and γ_n is compact. Using (3.36) and the fact that $(\eta, w)_{L^2} = (R\eta, w)_{L^2}$ for $w \in \gamma_n(\tilde{H})$, we have

$$\int_\Gamma \eta_0 B\eta_1 \, ds = \int_\Gamma \eta_0 \gamma_n \mathbf{u}[\eta_1] \, ds = \int_\Gamma (R\eta_0)(\gamma_n \mathbf{u}[\eta_1]) \, ds = -a(\mathbf{u}[\eta_0], \mathbf{u}[\eta_1]). \tag{3.57}$$

Since $a(\cdot,\cdot)$ is symmetric and coercive on $\tilde{H}$, B is self-adjoint and negative:

$$(\eta_0, B\eta_1)_{L^2} = (\eta_1, B\eta_0)_{L^2}, \qquad (\eta_0, B\eta_0)_{L^2} \le 0 \qquad \left(\eta_0, \eta_1 \in L^2(\Gamma)\right). \tag{3.58}$$

Note that $(\eta, B\eta)_{L^2}$ is related to the elastic energy stored in the grains:

$$E = \frac{1}{2} a\left(\mathbf{u}[\eta], \mathbf{u}[\eta]\right) = -\frac{1}{2}\int_\Gamma \eta B\eta \, ds \qquad \left(\eta \in L^2(\Gamma)\right). \tag{3.59}$$

Since $E = 0$ iff $\mathbf{u} \equiv 0$, and $\mathbf{u}[\eta] \equiv 0$ precisely when $\eta \in \gamma_n(H_d)$, we find that $\ker(B) = \gamma_n(H_d)$ as claimed. ∎

DEFINITION 3.22. *The operator S is defined to be the pseudoinverse of B.*

Remark 3.23. Since B is self-adjoint and compact, it has an orthonormal eigendecomposition $B = \sum_1^\infty \beta_k(\cdot, \chi_k)\chi_k$ with $(\beta_1 = \cdots = \beta_q = 0)$ and the remaining β_k forming an increasing sequence of negative numbers converging to zero. S is defined as $S = \sum_1^\infty \alpha_k(\cdot, \chi_k)\chi_k$, where $\alpha_k = 0$ for $k \le q$ and $\alpha_k = 1/\beta_k$ for $k > q$. Since S is defined with respect to an orthonormal basis, we know it is self-adjoint, densely defined, and negative, and its range is $\gamma_n(H_d)^\perp$. Note that the operators S and B satisfy $SB = R$, $BS = R\big|_{\mathcal{D}(S)}$.

DEFINITION 3.24. *A solution of the grain boundary displacement jump problem for a given $g \in \mathcal{D}(S)$ is a solution $\mathbf{u}$ of the normal stress problem with $\eta = Sg$, subject to the additional requirement that $\gamma_n \mathbf{u} = g$.*

THEOREM 3.25. *For any $g \in \mathcal{D}(S)$ there is a unique solution $\mathbf{u}(g)$ of the grain boundary displacement jump problem.*

Proof. Suppose $g \in \mathcal{D}(S)$. Since γ_n is injective on H_d and $\text{range}(I - R) = \gamma_n(H_d)$, there is a unique $\mathbf{u}_d[g] \in H_d$ such that $\gamma_n(\mathbf{u}_d[g]) = (I - R)g$. Clearly

$$\mathbf{u}(g) = \mathbf{u}_d[g] + \mathbf{u}[Sg] \tag{3.60}$$

is the desired solution, where $\mathbf{u}[Sg]$ is the unique solution in $\tilde{H}$ with normal stress Sg specified on Γ; see Proposition 3.12 and note that $\gamma_n(\mathbf{u}(g)) = (I - R)g + BSg = g$. ∎

Remark 3.26. In the degenerate case, the condition $\gamma_n \mathbf{u} = g$ removes the indeterminacy of the solution to the normal stress problem. As a result, the operator S truly maps g to the corresponding normal stress η, whereas B has nonphysical projections built into it for the convenience of being defined on all of $L^2(\Gamma)$.

Remark 3.27. The domain $\mathcal{D}(S)$ is quite complicated due to the variety of ways self-similar solutions of the Lamé equations can behave near grain boundary junctions; see [9, 12]. In particular, even for smooth functions η that are continuous at junctions, $g = B\eta$ generally will be discontinuous at junctions and exhibit infinite slopes. As a result, it would be very difficult to define weak solutions to the grain boundary displacement jump problem directly (without using the grain boundary normal stress problem) and to characterize those g for which the resulting normal stress η is meaningful in the trace sense. The above approach allows us to define S and derive its properties via the compact operator B, which avoids these complications.

4. Dynamics. In this section we show that the equation

$$\eta_t = SL\eta, \qquad \eta(0) = \eta_0, \tag{4.1}$$

generates an analytic semigroup $\{E_t : t \ge 0\}$ of bounded linear operators on $H^1(\Gamma)$. As mentioned previously, the solution $\eta(t)$ when the electromigration force is present

is then given by

$$\eta(t) = E_t(\eta_0 + \psi) - \psi. \tag{4.2}$$

The boundary conditions on $\eta(t) + \psi$ at junctions hold for $t > 0$ as a consequence of the analyticity of E_t and the properties of $\mathcal{D}(SL)$. We will also show that the evolution of grain growth is given by

$$g(t) = R_1 B\eta(t) + (I - R_1)g_0 + [(I - R_1)L\psi]t, \tag{4.3}$$

where R_1 is a projection with kernel of dimension $q = \dim\ker S$ (the degree of degeneracy of the grain boundary network). The term that grows linearly in time corresponds to a continual transport of material around the grains, leading to stress-free rigid body motions in each grain suggestive of continental drift in plate tectonics.

4.1. Semigroup theory. We briefly review the elements of semigroup theory we will need in what follows. A family $\{E_t : t \geq 0\}$ of bounded linear operators on a Banach space X is called a *strongly continuous semigroup* if

$$\begin{aligned} &\text{(i)} && E_{t+s} = E_t E_s \quad (t, s \geq 0), \\ &\text{(ii)} && E_0 = id_X, \\ &\text{(iii)} && t \mapsto E_t x \text{ is continuous on } [0, \infty) \text{ for each fixed } x \in X. \end{aligned} \tag{4.4}$$

If $\|E_t\| \leq 1$ for all $t \geq 0$, $\{E_t\}$ is called a *contraction semigroup*. The *infinitesimal generator* A of a strongly continuous semigroup $\{E_t\}$ is given by

$$Ax = \lim_{h \to 0^+} [E_h x - x]/h \qquad (x \in \mathcal{D}(A)), \tag{4.5}$$

where $\mathcal{D}(A)$ is the set of all $x \in X$ for which the limit exists. It can be proved [2] that $\mathcal{D}(A)$ is dense in X, that A on $\mathcal{D}(A)$ is a closed operator, and that for $x \in \mathcal{D}(A)$, $t \mapsto E_t x$ is continuously differentiable and satisfies

$$\frac{d}{dt} E_t x = AE_t x = E_t Ax \qquad (0 \leq t < \infty). \tag{4.6}$$

The semigroup $\{E_t\}$ is said to be differentiable if $E_t X \subset \mathcal{D}(A)$ for $t > 0$, in which case [2] it is infinitely differentiable and for each $t > 0$ the operators $E_t^{(n)}$ given by

$$E_t^{(n)} x := \frac{d^n}{dt^n} E_t x = A^n E_t x \tag{4.7}$$

are bounded and satisfy

$$E_t^{(n)} x = (E'_{t/n})^n x \qquad (t > 0). \tag{4.8}$$

A differentiable semigroup is said to be analytic if

$$\limsup_{t \to 0} t\|E'_t\| = \alpha < \infty, \tag{4.9}$$

which is equivalent [11] to having a holomorphic extension E_λ given locally by

$$E_\lambda x = \sum_{n=0}^{\infty} \frac{(\lambda - t)^n}{n!} E_t^{(n)} x \qquad \left(t > 0, \quad |\lambda - t| < \frac{t}{\alpha e}, \quad x \in X\right). \tag{4.10}$$

THEOREM 4.1. *If X is a Hilbert space and A is a closed, densely defined, negative, self-adjoint operator on X, then A is the infinitesimal generator of a contraction semigroup $\{E_t\}$ with holomorphic extension $\{E_\lambda : \operatorname{Re}\lambda > 0\}$, and $\alpha \leq e^{-1}$ in* (4.9).

Proof. See [7, 14]. □

4.2. The semigroup generated by SL. The main obstacle to solving (4.1) is that although S and L are each self-adjoint, they do not commute, and hence SL is not self-adjoint. If L were invertible, the obvious thing to do in this situation (see, e.g., [8]) would be to define a new variable $y = L^{\frac{1}{2}}\eta$, use Theorem 4.1 to obtain the solution $y(t)$ of the equation

$$y_t = L^{\frac{1}{2}} S L^{\frac{1}{2}} y, \qquad y(0) = y_0, \tag{4.11}$$

with $y_0 = L^{\frac{1}{2}}\eta_0$, and check that $\eta = L^{-\frac{1}{2}} y$ satisfies (4.1). Since L has a d dimensional kernel, we cannot directly obtain η from y in this way, and we will instead rely on the knowledge that $y(t) - y_0 \in \operatorname{ran}(L^{\frac{1}{2}} S L^{\frac{1}{2}})$ for all time while $\eta(t) - \eta_0 \in \operatorname{ran}(SL)$.

CONVENTION 4.2. *Generic elements of* $\ker(L)$ *and* $\ker(S)$ *will be denoted* e *and* h *so that the notation* $\{e, Gh\}$*, for example, represents the space* $\ker(L) \oplus G\ker(S)$.

Recall from (2.10) and (3.51) that we have defined $d = \dim\{e\}$, $q = \dim\{h\}$, and P and R as the orthogonal projections onto $\{e\}^\perp$ and $\{h\}^\perp$, respectively:

$$P = I - \sum_{k=1}^{d} (\cdot, e_k) e_k, \qquad R = I - \sum_{k=1}^{q} (\cdot, h_k) h_k. \tag{4.12}$$

By Theorem 3.9, we know $\{e\} \perp \{h\}$; hence P and R commute. Moreover, B is injective on $\{e\}$ (and G on $\{h\}$) since $\{e\} \cap \ker(B) = \{e\} \cap \{h\} = \{0\}$.

LEMMA 4.3. *The following identities hold:*

$$\begin{aligned} &\ker(SL) = \{e, Gh\}, \quad \ker(LS) = \{Be, h\}, \quad \ker(L^{\frac{1}{2}} S L^{\frac{1}{2}}) = \{e, G^{\frac{1}{2}} h\}, \\ &\operatorname{ran}(SL) = \{Be, h\}^\perp, \quad \operatorname{ran}(LS) = \{e, Gh\}^\perp, \quad \operatorname{ran}(L^{\frac{1}{2}} S L^{\frac{1}{2}}) = \{e, G^{\frac{1}{2}} h\}^\perp. \end{aligned} \tag{4.13}$$

Proof. SL is densely defined in $L^2(\Gamma)$ since $\mathcal{D}(S)$ is dense, G is bounded with range dense in $\{e\}^\perp$, and $\mathcal{D}(SL) = \{e\} \oplus G\mathcal{D}(S)$. Likewise $\mathcal{D}(LS) = \{h\} \oplus B\mathcal{D}(L)$ and $\mathcal{D}(L^{\frac{1}{2}} S L^{\frac{1}{2}}) = \{e\} \oplus G^{\frac{1}{2}}[\{h\} \oplus B\mathcal{D}(L^{\frac{1}{2}})]$ are dense in $L^2(\Gamma)$. Clearly, $\ker(SL) \supset \{e, Gh\}$. Since $\{h\} \subset \{e\}^\perp$ and LG is the identity on $\{e\}^\perp$, the only vectors mapped to $\{h\}$ by L belong to $\{e, Gh\}$, so the reverse inclusion also holds. A similar argument establishes $\ker(LS) = \{Be, h\}$. For $\ker(L^{\frac{1}{2}} S L^{\frac{1}{2}})$, we use

$$(x, L^{\frac{1}{2}} S L^{\frac{1}{2}} x) = 0 \quad \Leftrightarrow \quad -(|S|^{\frac{1}{2}} L^{\frac{1}{2}} x, |S|^{\frac{1}{2}} L^{\frac{1}{2}} x) = 0 \quad \Leftrightarrow \quad |S|^{\frac{1}{2}} L^{\frac{1}{2}} x = 0 \tag{4.14}$$

and argue as in the other two cases. The result $\operatorname{ran}(SL) \subset \ker(LS)^\perp$ follows from the fact that $(SL)^* = LS$, and $\operatorname{ran}(SL) \supset \{Be, h\}^\perp$ is a consequence of Lemma 4.9 below. Similar arguments give $\operatorname{ran}(LS)$ and $\operatorname{ran}(L^{\frac{1}{2}} S L^{\frac{1}{2}})$. ∎

Remark 4.4. Since $\{e\} \perp \{Gh\}$, $\{Be\} \perp \{h\}$ and $\{e\} \perp \{G^{\frac{1}{2}} h\}$, the kernels in (4.13) all have dimension $d + q = \dim\{e\} + \dim\{h\}$.

DEFINITION 4.5. *We define the (nonorthogonal) projections* P_1*,* R_1*, and* Q *on* $L^2(\Gamma)$ *via*

$$P_1 \text{ projects along } \{e\} \text{ onto } \{Be\}^\perp, \tag{4.15}$$

$$R_1 \text{ projects along } \{h\} \text{ onto } \{Gh\}^\perp, \tag{4.16}$$

$$Q \text{ projects along } \{e, Gh\} = \ker(SL) \text{ onto } \{Be, h\}^\perp = \operatorname{ran}(SL). \tag{4.17}$$

Remark 4.6. In general, if X and Y are finite dimensional subspaces of the same dimension such that $X \cap Y^\perp = \{0\}$, the projection along X onto $Y^\perp$ exists and is

given by $I-(\cdot,w_k)x_k$ (summation is implied). Here $\{x_k\}$ is a basis for X, $\{y_k\}$ is a basis for Y, $w_k=y_j\alpha_{jk}$, and $(x_i,y_j)\alpha_{jk}=\delta_{ik}$. To verify that P_1, R_1, and Q are well defined, we must check the condition $X\cap Y^\perp=\{0\}$.

Suppose $x\in\{e\}\cap\{Be\}^\perp$. Then $(x,Bx)=-(|B|^{\frac12}x,|B|^{\frac12}x)=0$, which implies $x\in\{h\}$. Since $\{e\}\perp\{h\}$, $x=0$ as required. An identical argument works for R_1.

Suppose $x\in\{e,Gh\}\cap\{Be,h\}^\perp$. Then there is $e_0\in\{e\}$ and $h_0\in\{h\}$ such that $x=e_0+Gh_0$. Since $x\perp\{h\}$ and $e_0\perp h_0$, we have $(x,h_0)=(Gh_0,h_0)=0$. Since G is self-adjoint and positive, this implies $h_0\in\{e\}$ so that $x=e_0+0$. But now we have $x\in\{e\}\cap\{Be\}^\perp$, which implies $x=0$ from the above argument.

Remark 4.7. Note that there are $w_k\in\{Be\}$ and $z_k\in\{Gh\}$ such that

$$P_1=I-\sum_{k=1}^{d}(\cdot,w_k)e_k,\qquad R_1=I-\sum_{k=1}^{q}(\cdot,z_k)h_k. \tag{4.18}$$

As a result, in addition to being bounded in $L^2(\Gamma)$, P_1 is also bounded as an operator on $H^1(\Gamma)$ since the e_k belong to this space. On the other hand, the L^2 adjoint $P_1^*=I-(\cdot,e_k)w_k$ is not necessarily defined on $H^1(\Gamma)$ due to the possibility of singularities in the derivative of w_k near junctions. Similarly, R_1^* is a projection in $H^1(\Gamma)$ while R_1 generally is not due to discontinuities in the h_k at junctions.

Remark 4.8. Q may be written $Q=P_1R_1^*$ since $\{e\}\perp\{Gh\}$ and $\{e\}\perp\{h\}$.

LEMMA 4.9. *The following diagrams are commutative in the sense that for each block* $X\underset{g}{\overset{f}{\rightleftarrows}}Y$ *we have* $f\circ g=id_Y$ *and* $g\circ f=id_{\mathcal{D}(f)}$*:*

(4.19)

$$\{e,G^{\frac12}h\}^\perp\underset{G^{\frac12}}{\overset{L^{\frac12}}{\rightleftarrows}}\{e,Gh\}^\perp\underset{R_1}{\overset{R}{\rightleftarrows}}\{e,h\}^\perp\underset{B}{\overset{S}{\rightleftarrows}}\{Be,h\}^\perp\underset{P_1}{\overset{P}{\rightleftarrows}}\{e,h\}^\perp\underset{G^{\frac12}}{\overset{L^{\frac12}}{\rightleftarrows}}\{e,G^{\frac12}h\}^\perp,$$

$$\{Be,h\}^\perp\underset{P_1}{\overset{P}{\rightleftarrows}}\{e,h\}^\perp\underset{G}{\overset{L}{\rightleftarrows}}\{e,Gh\}^\perp\underset{R_1}{\overset{R}{\rightleftarrows}}\{e,h\}^\perp\underset{B}{\overset{S}{\rightleftarrows}}\{Be,h\}^\perp. \tag{4.20}$$

Proof. P and P_1 both project along $\{e\}$, so $PP_1=P$ and $P_1P=P_1$. Since $\{e\}\perp\{h\}$, both projections leave $\{h\}^\perp$ invariant. Since $\mathrm{ran}(P)=\{e\}^\perp$ and $\mathrm{ran}(P_1)=\{Be\}^\perp$, the blocks involving P and P_1 are commutative. Identical arguments may be used for the blocks involving R and R_1.

Note that if $(x,Gh)=0$, then $(Gx,h)=0$; i.e., G maps $\{Gh\}^\perp$ into $\{h\}^\perp$. Since LG is the identity on $\{e\}^\perp$ (recall $\mathcal{D}(L)=\mathrm{ran}(G)\oplus\{e\}$) and GL is the identity on $\{e\}^\perp\cap\mathcal{D}(L)$, the blocks involving L and G are commutative. Identical arguments may be used for the remaining blocks. ∎

DEFINITION 4.10. *We say that* T *is the* pseudoinverse *of the bounded operator* K *on the Hilbert space* H *if there are closed subspaces* X *and* Y *(not necessarily orthogonal) such that* $H=X\oplus Y$, $\ker(T)=X=\ker(K)$, *and*

$$TKy=y\quad(y\in Y),\qquad KTy=y\quad(y\in Y\cap\mathcal{D}(T)). \tag{4.21}$$

In particular, we require $\mathrm{ran}(K)\subset\mathcal{D}(T)$.

LEMMA 4.11. *Such a* T *is closed.*

Proof. First we claim that $\mathrm{ran}(T)=Y$. Clearly, (4.21) implies $\mathrm{ran}(T)\supset Y$. To prove the reverse inclusion, suppose $x_1+y_1=T(x_2+y_2)$ with $x_i\in X$, $y_i\in Y$. Then $Ky_1=KTy_2=y_2$, so $y_1=TKy_1=Ty_2=x_1+y_1$, which implies $x_1=0$ as required.

Now suppose $a_k \to a$, $Ta_k \to b$. We must show $Ta = b$. Note that $b \in Y$ since each $Ta_k \in Y$ and Y is closed. Decompose $a_k = x_k + y_k$ and $a = x + y$ using $H = X \oplus Y$. Then $y_k \to y$ since the projection along X onto Y is continuous. We also know $y_k = KTy_k = KTa_k \to Kb$ since K is continuous. Thus $y = Kb$ and $a = x + y \in \mathcal{D}(T)$. Finally, $Ta = Ty = TKb = b$ since $b \in Y$. ∎

Remark 4.12. If there is an eigenbasis for K, then it is an eigenbasis for both operators, and the eigenvalues are reciprocal or zero. When K is not self-adjoint, this definition differs from the usual definition in linear algebra that T and K should have the same SVD bases (exchanging left and right singular vectors) with reciprocal (or zero) singular values. The current definition is more useful for eigenvalue problems while the usual one is more useful for least squares problems. The definitions coincide when T and K are self-adjoint.

THEOREM 4.13. *The following pseudoinverse relationships hold:*

$$L^{\frac{1}{2}} S L^{\frac{1}{2}} = \operatorname{pinv}(G^{\frac{1}{2}} Q^* B Q G^{\frac{1}{2}}), \tag{4.22}$$

$$SL = \operatorname{pinv}(QGBQ), \tag{4.23}$$

$$LS = \operatorname{pinv}(Q^* B G Q^*). \tag{4.24}$$

Proof. Since $SR = S$ and $LP = L$, the left-to-right compositions in (4.19) and (4.20) are $L^{\frac{1}{2}} S L^{\frac{1}{2}}$ and SL, respectively. Because P_1 leaves $\{h\}^\perp$ invariant, Q and P_1 agree on $\{h\}^\perp$. Likewise Q^* and R_1 agree on $\{e\}^\perp$, so the right-to-left compositions are $G^{\frac{1}{2}} Q^* B Q G^{\frac{1}{2}}$ and QGQ^*B, respectively.

Clearly, $K := G^{\frac{1}{2}} Q^* B Q G^{\frac{1}{2}}$ annihilates $X := \{e, G^{\frac{1}{2}} h\} = \ker(L^{\frac{1}{2}} S L^{\frac{1}{2}})$, and (4.19) ensures that (4.21) holds with $T := L^{\frac{1}{2}} S L^{\frac{1}{2}}$, $Y := \{e, G^{\frac{1}{2}} h\}^\perp$ as required.

The operator QGQ^*B does not have the same kernel as $T := SL$; however, this is easily corrected using $K := QGQ^*BQ$ instead. We then have $\ker(K) = \ker(T) = \{e, Gh\} =: X$ by (4.13) and (4.17). Equation (4.20) implies that (4.21) holds with $Y := \{Be, h\}^\perp$, which complements X in $L^2(\Gamma)$ since Q is a well-defined projection. Finally, by Remark 4.8 and the identities $R_1^* G R_1 = R_1^* G = G R_1$, $P_1^* B P_1 = P_1^* B = B P_1$, it follows that $QGQ^*BQ = QGBQ$. The proof for LS is similar. ∎

LEMMA 4.14. *Equation* (4.11) *generates an analytic contraction semigroup* $\{\tilde{E}_t : t \geq 0\}$ *of bounded linear operators on* $L^2(\Gamma)$. *For each* $t \geq 0$, $P\tilde{E}_t P = \tilde{E}_t P$.

Proof. We showed that $L^{\frac{1}{2}} S L^{\frac{1}{2}}$ has dense domain in the proof of Lemma 4.3. It is closed by Lemma 4.11 and Theorem 4.13, self-adjoint since L and S are self-adjoint, and negative since S is negative:

$$(x, L^{\frac{1}{2}} S L^{\frac{1}{2}} x) = (L^{\frac{1}{2}} x, S L^{\frac{1}{2}} x) \leq 0. \tag{4.25}$$

Theorem 4.1 may therefore be applied to conclude that $L^{\frac{1}{2}} S L^{\frac{1}{2}}$ is the generator of an analytic contraction semigroup $\{\tilde{E}_t : t \geq 0\}$ of bounded linear operators. Since $\operatorname{ran}(L^{\frac{1}{2}} S L^{\frac{1}{2}}) \subset \{e\}^\perp$, for $y_0 \in L^2(\Gamma)$ we have

$$(\tilde{E}_t y_0, e_k) = (\tilde{E}_0 y_0, e_k) + \int_0^t (L^{\frac{1}{2}} S L^{\frac{1}{2}} \tilde{E}_s y_0, e_k)\, ds = (y_0, e_k). \tag{4.26}$$

Hence $\tilde{E}_t$ leaves $\{e\}^\perp$ invariant, and $P\tilde{E}_t P = \tilde{E}_t P$ as claimed. ∎

THEOREM 4.15. *The family* $\{E_t : t \geq 0\}$ *given by*

$$E_t = (I - P_1) + P_1 G^{\frac{1}{2}} \tilde{E}_t L^{\frac{1}{2}} \tag{4.27}$$

is an analytic semigroup in $H^1(\Gamma)$. Its infinitesimal generator is SL.

Proof. Since $G^{\frac12}$ is bounded from L^2 to H^1, $L^{\frac12}$ is bounded from H^1 to L^2, and P_1 is bounded in H^1, there is a $C>0$ such that $\|P_1G^{\frac12}\tilde E_tL^{\frac12}\|_{H^1}\le C\|\tilde E_t\|_{L^2}$; therefore, each E_t is bounded in $H^1(\Gamma)$. Property (4.4)(iii) follows similarly: pick $x\in H^1$, and let $y=L^{\frac12}x$; then we have

$$\|(E_t-E_s)x\|_{H^1}=\|P_1G^{\frac12}(\tilde E_t-\tilde E_s)y\|_{H^1}\le C\|(\tilde E_t-\tilde E_s)y\|_{L^2}\underset{t\to s}{\longrightarrow}0. \tag{4.28}$$

Properties (4.4)(i) and (4.4)(ii) follow immediately from (4.27) and the corresponding properties of $\tilde E$, using the relations

$$P_1P=P_1,\quad PP_1=P,\quad L^{\frac12}=L^{\frac12}P,\quad G^{\frac12}L^{\frac12}=P=L^{\frac12}G^{\frac12},\quad P\tilde E_sP=\tilde E_sP. \tag{4.29}$$

The analyticity may be seen by computing

$$\limsup_{t\to0}t\|E_t'\|_{H^1}\le C\limsup_{t\to0}t\|\tilde E_t'\|_{L^2}<\infty. \tag{4.30}$$

To prove that the generator of E_t is SL, we first note that

$$L^{\frac12}E_t=L^{\frac12}P_1G^{\frac12}\tilde E_tL^{\frac12}=P\tilde E_tL^{\frac12}=\tilde E_tL^{\frac12} \tag{4.31}$$

and compute

$$E_t'=P_1G^{\frac12}\big(L^{\frac12}SL^{\frac12}\tilde E_t\big)L^{\frac12}=P_1PSL^{\frac12}\big(L^{\frac12}E_t\big)=P_1SLE_t=SLE_t. \tag{4.32}$$

∎

Proposition 4.16. *There is a Riesz basis $\{\phi_k\}$ for $H^1(\Gamma)$ and a nonincreasing, unbounded sequence of numbers $\lambda_k\le0$ such that $SL\phi_k=\lambda_k\phi_k$.*

Proof. Since $G^{\frac12}Q^*BQG^{\frac12}$ is self-adjoint and compact, the spectral theorem gives an L^2 orthonormal basis of eigenfunctions $\{\varphi_k\}_{k=1}^\infty$, which by Theorem 4.13 is also an eigenbasis of $L^{\frac12}SL^{\frac12}$: φ_k is either in the kernel of both operators, or it is an eigenfunction of each with reciprocal eigenvalues. Since S is negative, the eigenvalues λ_k of $L^{\frac12}SL^{\frac12}$ satisfy $\lambda_k\le0$. Since $L^{\frac12}SL^{\frac12}$ commutes with P, we may assume the φ_k are also eigenfunctions of P (with eigenvalue 0 or 1). Define

$$\phi_k=\begin{cases}\varphi_k, & P\varphi_k=0,\\ P_1G^{\frac12}\varphi_k & \text{otherwise.}\end{cases} \tag{4.33}$$

In the first case we have $SL\phi_k=0$. In the second, we obtain

$$SLP_1G^{\frac12}\varphi_k=SL^{\frac12}\varphi_k=P_1SL^{\frac12}\varphi_k=P_1G^{\frac12}L^{\frac12}SL^{\frac12}\varphi_k=\lambda_kP_1G^{\frac12}\varphi_k. \tag{4.34}$$

The ϕ_k are related to the φ_k via

$$\phi_k=\big[(I-P)+P_1G^{\frac12}\big]\varphi_k,\qquad \varphi_k=\big[(I-P_1)+L^{\frac12}\big]\phi_k. \tag{4.35}$$

Since $[I-P+P_1G^{\frac12}]$ is bounded from $L^2(\Gamma)$ to $H^1(\Gamma)$ and its inverse $[I-P_1+L^{\frac12}]$ is bounded in the other direction, they are isomorphisms. Thus the ϕ_k form a Riesz basis (a basis equivalent to an orthonormal basis [6]) for $H^1(\Gamma)$ as claimed. ∎

Remark 4.17. Equation (4.27) could also have been written

$$E_t=[I-P+P_1G^{\frac12}]\,\tilde E_t\,[I-P_1+L^{\frac12}]. \tag{4.36}$$

Remark 4.18. For $\eta_0 \in H^1(\Gamma)$, the coefficients in the expansion $\eta_0 = \sum_k a_k \phi_k$ can be determined via

$$a_k = ([I - P_1 + L^{\frac{1}{2}}]\eta_0, \varphi_k)_{L^2} = (\eta_0, \phi_k^*)_{L^2}, \qquad \phi_k^* = [I - P_1^* + L^{\frac{1}{2}}]\varphi_k. \tag{4.37}$$

The ϕ_k^* are eigenfunctions of LS with eigenvalues λ_k since $LS\phi_k^* = [(SL - P_1 SL)^* + LSL^{\frac{1}{2}}]\varphi_k = \lambda_k L^{\frac{1}{2}}\varphi_k = \lambda_k \phi_k^*$. They belong to $L^2(\Gamma)$ but need not belong to $H^1(\Gamma)$ due to possible singularities in $\partial_s \phi_k^*$ at junctions. For $\eta_0 \in H^1(\Gamma)$ the expansions

$$\eta_0 = \sum_{k=1}^{\infty} a_k \phi_k, \qquad E_t \eta_0 = \sum_{k=1}^{\infty} a_k e^{\lambda_k t}\phi_k, \qquad a_k = (\eta_0, \phi_k^*)_{L^2(\Gamma)}, \tag{4.38}$$

hold in $H^1(\Gamma)$. Note that the L^2 norm of ϕ_k^* diverges as $k \to \infty$, but when $\eta_0 \in H^1(\Gamma)$, the inner products a_k in (4.38) do not; they are square summable.

Remark 4.19. The expansions (4.38) lead to a useful numerical method in which the ϕ_k, ϕ_k^*, and λ_k are computed by approximating the pseudoinverse $\mathrm{pinv}(SL) = QGBQ$ using a singularity-capturing least squares finite element method; see [12, 9].

PROPOSITION 4.20. $\lim_{t\to\infty} E_t = I - Q$ *in norm.*

Proof. Recall that $\dim\ker(SL) = d + q$ so that $\lambda_1 = \cdots = \lambda_{d+q} = 0$. Since $\{\phi_k\}_{k=1}^{d+q}$ is a basis for $\mathrm{range}(I - Q)$, we have

$$[E_t - (I - Q)]\eta_0 = \sum_{k=d+q+1}^{\infty} a_k e^{\lambda_k t}\phi_k. \tag{4.39}$$

Since the mapping $\eta_0 \mapsto \langle a_k\rangle_{k=1}^{\infty}$ with $a_k = (\eta_0, \phi_k^*)_{L^2}$ is an isomorphism from $H^1(\Gamma)$ to l^2, there is a constant C such that

$$\|(E_t - I + Q)\eta_0\|_{H^1} \le Ce^{\lambda^* t}\|\eta\|_{H^1} \qquad (t \ge 0,\ \eta_0 \in H^1(\Gamma)) \tag{4.40}$$

with $\lambda^* = \lambda_{d+q+1} < 0$. Thus $\|E_t - (I - Q)\|_{H^1} \le Ce^{\lambda^* t} \to 0$ as $t \to \infty$ as claimed. ∎

Remark 4.21. Since E_t is an operator on $H^1(\Gamma)$ and the formula for the evolution of normal stress is given by

$$\eta(t) = E_t(\eta_0 + \psi) - \psi, \tag{4.41}$$

we should verify that ψ belongs to $H^1(\Gamma)$. This is done in the companion paper [13].

Remark 4.22. Since E_t is analytic, we have $\mathrm{ran}(E_t) \subset \mathcal{D}(SL)$ for all $t > 0$. Therefore $\eta(t)$ in (4.41) has the property that

$$\eta(t) + \psi \in \mathcal{D}(L) \qquad (t > 0). \tag{4.42}$$

Thus although ψ does not necessarily satisfy zero flux boundary conditions at junctions, the normal stress η immediately compensates so that for all $t > 0$, flux balance holds. As long as there is a displacement jump $g(t)$ compatible with the evolution of $\eta(t)$, we have proved that the grain boundary diffusion problem is well posed.

4.3. The evolution of *g*. In the nondegenerate case, the evolution of g is easily determined from the evolution of η in (4.41) via

$$g(t) = B\eta(t) \qquad \text{(nondegenerate case)}. \tag{4.43}$$

The situation becomes much more complicated (and rather interesting) in the degenerate situation where the subspace $\{h\} = \ker(S) = \ker(B)$ is nontrivial. In that case, each function in $\{h\}$ is a growth mode which is not suppressed by the grain boundary diffusion process. If such a mode h is activated by ψ, it will grow linearly in time without bound, as will the corresponding $\mathbf{u} \in H_d$ such that $\gamma_n \mathbf{u} = h$; see Definition 3.5. The nonlinear picture in which $\mathbf{u}$ is replaced by a collection of genuine (as opposed to infinitesimal) rigid body motions on each grain resembles continental drift in plate tectonics, at least superficially. The steady state stress distribution does not fully cancel the flux due to electromigration, and material is continually transported around the participating grains, causing them to drift in order to avoid misfit with their neighbors as material is removed from one side and deposited on the other.

THEOREM 4.23. *The evolution of g is given by*

$$g(t) = R_1 B\eta(t) + (I - R_1)g_0 + [(I - R_1)L\psi]t. \tag{4.44}$$

Proof. Recall that the projections R and R_1 may be written

$$R = I - \sum_{k=1}^{q} (\cdot, h_k)h_k, \quad R_1 = I - \sum_{k=1}^{q} (\cdot, z_k)h_k \quad \big(h_k \in \{h\}, z_k \in \{Gh\}\big). \tag{4.45}$$

Note that $(I - R_1)L = \sum_{k=1}^{q} (\cdot, Lz_k)h_k$ is actually a bounded operator on $L^2(\Gamma)$, so its domain may be extended from $\mathcal{D}(L)$ to $L^2(\Gamma)$. Since $\ker(S) = \{h\}$, we see that $S(I - R_1) = 0$. Therefore

$$Sg = SB\eta = R\eta = \eta, \tag{4.46}$$

where the last step follows from the fact that $\eta_0 := Sg_0 \in \operatorname{ran}(R)$ and

$$\eta_t = SL(\eta + \psi) \quad \Rightarrow \quad \eta - \eta_0 \in \operatorname{ran}(SL) \subset \operatorname{ran}(R). \tag{4.47}$$

We next use $R_1 R = R_1$ and $BS = R\big|_{\mathcal{D}(S)}$ to conclude that

$$g(0) = R_1 BSg_0 + (I - R_1)g_0 = g_0. \tag{4.48}$$

Finally, we check that g solves the evolution equation $g_t = L(Sg + \psi)$:

$$\begin{aligned} g_t &= R_1 BSL(\eta + \psi) + (I - R_1)L\psi \\ &= R_1 L(Sg + \psi) + (I - R_1)L\psi \\ &= L(Sg + \psi) - [(I - R_1)L](Sg + \psi - \psi) \\ &= L(Sg + \psi). \end{aligned} \tag{4.49}$$

In the last step, we used the fact that $(I - R_1)LSg = 0$ since $\operatorname{ran}(LS) \subset \{Gh\}^{\perp} = \ker(I - R_1)$ by (4.13) and (4.16). In the second-to-last step we were careful not to break up $(I - R_1)L$ when acting on ψ since the latter may not belong to the domain of L. In contrast, the function $(Sg + \psi)$ belongs to $\mathcal{D}(L)$ for $t > 0$, as discussed in Remark 4.22. ∎

Remark 4.24. Once $g(t)$ is known, the stress and displacement fields inside the grains are uniquely determined as the solution to the grain boundary displacement jump problem; see Definition 3.24 and Theorem 3.25.

5. Conclusion. The stress-driven grain boundary diffusion problem involves coupling many different equations and phenomena that lead to interesting behavior due to the interplay between nonlocality, singular behavior, and complex geometry. By posing the problem as an evolution of functions defined on the grain boundary, we were able to use methods of semigroup theory to answer fundamental questions of existence, uniqueness, and appropriateness of boundary conditions. In the process, we discovered a class of degenerate grain boundaries that exhibit interesting behavior.

Placing this problem back into the larger model, which includes void and vacancy evolution, grain boundary sliding, etc., it would be interesting to study the behavior of the solution in the vicinity of a junction where a void meets a grain boundary. Here again, questions of appropriate boundary conditions arise, thermodynamic arguments are murky, and singularities in the stress tensor and electric field together with the stiffness inherent in grain boundary diffusion and curvature-driven surface diffusion make the problem difficult to attack theoretically and numerically.

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