Stable Disarrangement Phases Arising from Expansion/Contraction or from Simple Shearing of a Model Granular Medium

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Abstract

¹A principal challenge in modelling granular media is to connect the macroscopic deformation of the aggregate of grains with the average deformation of a small number of individual grains. We used in previous research the two-scale geometry of structured deformations (g, G) and the theory of elastic bodies undergoing disarrangements (non-smooth submacroscopic geometrical changes)to obtain an algebraic tensorial consistency relation between the macroscopic deformation F = gradg and the grain deformation G, as well as an accommodation inequality $detF \ge detG > 0$ that guarantees that the aggregate provides enough room at each point for the deformation of the grains. These two relations determine all of the disarrangement phases G corresponding to a given F. We use the term stable disarrangement phase to denote a grain deformation G

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that minimizes the stored energy density for the aggregate $\psi(G')$ among all the disarrangement phases G' corresponding to F.

In this article we determine for a model aggregate and for two familiar families of macroscopic deformation – simple shearing and uniform expansion/contraction – all of the stable disarrangement phases of the model aggregate, as well as the corresponding connections between aggregate deformation and grain deformation. We showed in an earlier article that each stable disarrangement phase of this model aggregate cannot support tensile tractions, and our present, more detailed, results for simple shearing and for uniform expansion/contraction confirm that no-tension property of stable disarrangement phases for the model granular medium.

1 Introduction

A principal challenge in modelling multiscale phenomena in continua is that of describing the coupling between macroscopically observed geometrical changes and submacroscopically occurring geometrical changes. In this article we study in the setting of the multiscale geometry of structured deformations [1] the manner in which the macroscopic deformation of an aggregate of small elastic bodies that constitute a granular medium can be related to the submacroscopic deformation of the pieces of the aggregate. (Here, we use the terms "elastic aggregate" and "granular medium" synonymously.) Structured deformations provide an appropriate setting, because they entail purely geometrical fields gand G that distinguish between the macroscopic deformation of a continuum and the smooth geometrical changes that occur at submacroscopic length scales. In the case of elastic aggregates, we may think of the point mapping g as providing the macroscopic geometrical changes of the aggregate, as a whole, and we may think of the tensor field G as providing a measure of the average geometrical changes of individual pieces (or grains) of the aggregate. The theory of structured deformations then justifies calling the field $M = \nabla g - G$ the deformation due to disarrangements, i.e., due to submacroscopic slips and separations among the pieces of the aggregate. We emphasize in this paper the case in which the aggregate undergoes a given, homogeneous deformation g with gradient $\nabla g = F = const$. while all of the pieces of the aggregate undergo a sequence of piecewise homogeneous deformations whose gradients, when averaged over small subbodies, converge to the constant tensor field G.

A previously formulated theory [2] of elastic bodies undergoing disarrangements provides the *consistency* relation

$$D_G\Psi(G,M)(F^T - G^T) + D_M\Psi(G,M)F^T = 0,$$

a tensorial relation involving the fields $F = \nabla g$, G, M = F - G as well as the partial derivatives $D_G \Psi$ and $D_M \Psi$ of the Helmholtz free energy response Ψ of the body. The theory [2] also provides the accommodation inequality, $0 < \det G \leq \det F$, that guarantees that the macroscopic deformation F provides enough volume to accommodate the submacroscopic geometrical changes associated with G. Together the consistency relation and accommodation inequality determine which tensors G are compatible with a given macroscopic deformation gradient F. In [3], [20] we restricted attention to the case of *purely dissipative disarrangements* for which Ψ does not depend upon the disarrangement tensor M, so that the consistency relation reduces to $D\Psi(G)(F^T - G^T) = 0$. In this context, we defined in [20] a *disarrangement phase* corresponding to F to be a tensor G that satisfies both the consistency relation and the accommodation inequality for the given F. Examples that we give in this paper and have given elsewhere [2], [3], [20] show that typically there are multiple disarrangement phases corresponding to a given macroscopic deformation gradient F, and it is important to single out those disarrangement phases that are energetically favorable. Accordingly, we defined in [20] a stable disarrangement phase corresponding to F to be a disarrangement phase Gcorresponding to F that minimizes the Helmholtz free energy among all disarrangement phases corresponding to F. Our specific goals in this paper for a familiar two-parameter class of free energy responses $\Psi_{\alpha\beta}$ are:

- to determine all of the stable disarrangement phases corresponding to homogeneous expansions/contractions,
- to determine all of the stable disarrangement phases corresponding to simple shear,
- to describe in each of the two bullets above the relationship between the macroscopic deformation F = ∇g of the aggregate and the deformation G of the pieces of the aggregate.



Figure 1: Standard phases and disarrangement phases.

We illustrate now by means of two idealized, one-dimensional, isothermal stress-extension curves the idea of a disarrangement phase and compare it with the familiar notion of "phase of an elastic body". For the left-hand curve in Figure 1, the stress T is a (single-valued) function of the extension e with the property that, for some values of stress, there are more than one value of extension that produce that stress. For example, the stress T_0 can be achieved at three different values of the extension, and it is customary to refer to the three values of e corresponding to T_0 as phases of the elastic continuum corresponding to the stress T_0 . In this standard notion of phase, different phases may be distinguished by differences in the macroscopic deformation of the body, and an important goal in the study of phases for continua is that of providing contexts in which coexistent phases, even fine mixtures of such phases, can be described and simulated.

By contrast, the stress-extension curve on the right of the figure does not provide a single stress value T for each extension e, and we may fix the extension at the value e_0 and consider the three values of stress compatible with e_0 as corresponding to distinct phases of the material. Clearly, the macroscopic extension of the body cannot be used to distinguish among these phases, and it is natural to explore the possibility that disarrangements, i.e., non-smooth geometrical changes at submacroscopic length scales, may be used to distinguish among these phases. For both notions of "phase" illustrated here, one typically encounters a multiplicity of possible phases available to a given material, and an appropriate selection principle in the form of a stability criterion is required in order to narrow the list of competing phases. Our notion of stable disarrangement phase embodies this idea, is in accord with a notion of "submacroscopically stable equilibria of elastic bodies" introduced in [3], and is studied here in a fully three dimensional context for aggregates of elastic bodies.

In Section 2 we review the aspects of structured deformations and of the field theory "elasticity with disarrangements" [2] required for the present study.

The constitutive properties of the elastic aggregates are specified by means of the free energy response function Ψ , which is assumed not to depend upon the disarrangement tensor M = F - G, so that the disarrangements for the aggregates under considerationd do not result in the storage of energy and may be described as "purely dissipative." The field relations, including the consistency relation and the accommodation inequality, are given at the beginning of Section 2, and in Remark 1 we use the consistency relation to provide an inequality relating the energy when G = F to that when G differs from F by a rank-one tensor. In Section 2.1 we recall from [20] the definition of "disarrangement phase corresponding to F" as well as the notion of "compact phase" (disarrangement-free phase) and, for a slightly less general class of aggregates, the notion of "loose phases" (stress-free phases) of an aggregate. In the compact phase, the disarrangement tensor M vanishes, so that the pieces of the aggregate deform precisely as the aggregate through the macroscopic deformation gradient, i.e., $G = F = \nabla g$. In the loose phases, the pieces of the aggregate achieve a stress-free, energy minimizing state of deformation in which G is a scalar times an arbitrary rotation tensor. The accommodation inequality shows that loose phases can only be present when the volume change $\det F$ of the macroscopic deformation is sufficiently large.

The notion of a "stable disarrangement phase" as an energy-minimizing disarrangement phase [20] is reviewed in Section 2.2, and the notions of compact phase and loose phases are reexamined in light of this notion of material stability. Because for a broad class of free energies disarrangements of rank one cannot increase the free energy, the class of macroscopic deformations for which the compact phase is a stable disarrangement phase may be viewed as being rather limited.

Section 2.3 provides a review from earlier studies [20], [7], [3] of the two-

parameter class of free energy response functions $\Psi_{\alpha\beta}$ (with α and β "elastic constants") widely studied in the literature (see, for example, [19], Section 4.10). In Section 2.4 we record, for a given but arbitrary deformation gradient F, the complete catalog obtained in [20] of solutions of the consistency relation when $\Psi = \Psi_{\alpha\beta}$. These solutions G naturally form four categories: "compact," "plane-stress," "uniaxial stress." and "stress-free," the last three categories are identified according to the nature of the stress response S that is calculated for each category of solutions. Because the consistency relation can be written in the tensorial form $SM^T = 0$, the disarrangement tensors M = F - G for these categories turn out to have ranks 0, at most 1, at most 2, and at most 3, respectively.

In Section 2.5 we describe a procedure for finding the stable disarrangement phases corresponding to an arbitrary macroscopic deformation gradient F. For the free energy response $\Psi_{\alpha\beta}$, we carry out in Sections 3 this procedure in detail for the one parameter family $F = \lambda^{1/2} I$ of uniform expansions/contractions, and in Section 4 for the one-parameter family $F = I + \mu a \otimes b$ of simple shears. We obtain a complete list in Section 3 of the stable disarrangement phases corresponding to $F = \lambda^{1/2} I$, and in Section 4.5 a complete list of the stable disarrangement phases corresponding to $F = I + \mu a \otimes b$, conveniently described in terms of the maximum principal stretch $\lambda := 1 + (\mu^2 + |\mu| (\mu^2 + 4)^{1/2})/2 > 1$ for $\mu \neq 0$. The availability of these lists in the cases of expansion or contraction and in the case of simple shear provides detailed and specific insights into the dependence of G upon F when G is a stable disarrangement phase, and provides in Figures 2 and 5 partitions of the $\lambda - r$ plane into regions in each of which only one stable disarrangement phase (or, perhaps, only one class of equivalent phases) may arise. Figures 2 and 5 are counterparts of phase diagrams familiar in the study of standard phases of elastic bodies. For the stable disarrangement phases identified in Section 4.5 we are able to determine in Section 4.6 detailed connections between, on the one hand, the principal stretches and directions for F and, on the other, the principal stretches and directions for G. (The stable disarrangement phases found in Section 3 consist only of the compact phase and the loose phase for which the nature of G and its relationship to F were provided already in Section 2.1.)

The explicit results that we obtain here show that, for the two classes of macroscopic deformation gradients F studied in Sections 3 and 4, the stable disarrangement phases corresponding to F never result in tensile tractions within the body. These conclusions confirm the result established in Part II of [20] for arbitrary F: stable disarrangement phases associated with $\Psi_{\alpha\beta}$ cannot support tensile tractions. This property comes into play in Sections 3 and 4 where, for each given value of the ratio $r = \alpha/\beta$, there is a particular value $\hat{\lambda}(r)$ of the stretch parameter λ at which one of the principal stresses arising for the compact phase passes from negative values through zero to positive values as λ increases through $\hat{\lambda}(r)$, and stability of the compact phase thereby is lost. This loss of stability of the compact phase occurs in spite of the fact that the free energy $\Psi_{\alpha\beta}$ is smooth and rank-one convex. In particular, $\Psi_{\alpha\beta}$ satisfies the Legendre-Hadamard condition and, hence, does not admit material instabilities associated with loss of ellipticity ([13],[14], [16], [17], [18]).

We note that, for the stable plane-stress phase corresponding to the simple shear $F = I + \mu a \otimes b$, the free energy depends only upon the elastic constants α and β and not upon the amount of macroshear μ . This fluid-like behavior stands in contrast to the solid-like dependence of the free energy upon μ for the compact phase, and this result is in agreement with the observed ability of aggregates to exhibit both solid-like and fluid-like behavior [7], [8], [9], [10].

Our detailed results also include information about disarrangement phases

that lose the competition for the status of minima of the energy. Although energetically less favorable than their stable competitors, these unstable but in some cases energetically stationary disarrangement phases will play a role in the solution of boundary-value problems in the statics of elastic aggregates. In particular, boundary tractions computed from stresses arising in stable disarrangement phases may not agree with prescribed boundary tractions, as is the case for the loose phase in the presence of non-zero prescribed boundary tractions, thereby necessitating the formation of zones of unstable disarrangement phases near the boundary.

2 Summary of concepts and results from earlier studies

The multiscale geometry provided by structured deformations [1] has been applied [7] to describe moving phase interfaces in a granular medium composed of small elastic bodies that can deform individually in a manner that differs from the macroscopic deformation of the continuum. In [20] we specialized that description to a body that does not evolve in time, so that geometrical changes of the granular medium may be described by structured deformations (g, G). Each such structured deformation provides the macroscopic deformation $g: \mathcal{B} \longrightarrow \mathcal{E}$ mapping points X in the body \mathcal{B} injectively into Euclidean space \mathcal{E} as well as the deformation without disarrangements $G: \mathcal{B} \longrightarrow Lin$ mapping points X in the body formation of structured deformation of pieces of the granular medium. The definition of structured deformation includes the requirement that the fields g and G satisfy the accommodation inequality [1] at

each point X in the body:

$$0 < m < \det G(X) \le \det \nabla g(X). \tag{1}$$

Here, m is a positive number that does not depend upon X, ∇g is the classical derivative of the macroscopic deformation, and det denotes the determinant. This inequality reflects the idea that the macroscopic deformation should provide enough room to accommodate all of the pieces of the aggregate without causing interpenetration of matter.

The ability of the pieces of the aggregate to deform differently from the aggregate, itself, gives rise to slips and separations among the individual pieces called *disarrangements*. The accomodation inequality (1) can be used to prove the Approximation Theorem [1]: there exists a sequence $n \mapsto f_n$ of injective, piecewise-smooth mappings of the body into Euclidean space such that

$$g = \lim_{n \to \infty} f_n$$
 and $G = \lim_{n \to \infty} \nabla f_n$ (2)

where for present purposes the sense of convergence in the two limits need not be made explicit. Thus G, as a limit of classical derivatives, reflects at the macrolevel the smooth deformation away from any submacroscopic sites of disarrangements associated with the piecewise smooth approximates f_n . In addition, it has been shown [1], [11] that the tensor field

$$M = \nabla g - G \tag{3}$$

captures the average of the submacroscopic separations and slips embodied in the jumps of the approximates f_n , and we are justified in calling M the *defor*mation due to disarrangements. The piecewise smooth approximations f_n may be viewed as snapshots of the deforming aggregate taken with magnification sufficient to reveal the individual pieces of the aggregate.

We note that general elastic bodies undergoing disarrangements can store energy through both the deformation without disarrangements G and the deformation due to disarrangements M [2]. In order to specialize to the situation in which the slips and separations between pieces of the aggregate are purely dissipative, i.e., do not themselves contribute to the stored energy, it was assumed in [7] that the Helmholtz free energy field ψ for the aggregate is determined entirely by the deformation without disarrangements G, which at each point Xin the reference configuration amounts to the relation:

$$\psi(X) = \Psi(G(X)) \tag{4}$$

where Ψ is a smooth constitutive function, and $\psi(X)$ is the free energy per unit volume in the reference configuration. The constitutive equation (4) for an aggregate undergoing purely dissipative disarrangements can be derived from the assumption that (i) the energy associated with the piecewise smooth approximations f_n has no interfacial term and that (ii) the convergence in (2) is essentially uniform and Ψ is continuous. (See [12], Part Two, Section 2 for the supporting mathematical reasoning). This amounts to assuming that each piece of the aggregate is an elastic body with energy density response Ψ and that no energy is stored when pieces of the aggregate rotate, separate, or slide relative to one another.

The general field equations for elastic bodies undergoing disarrangements [2] reduce in the present, statical context and in the presence of purely dissipative disarrangements to the system

$$\operatorname{div} D\Psi(G) + b = 0 \tag{5}$$

$$D\Psi(G)(\nabla g - G)^T = 0 \tag{6}$$

$$0 < \det G \le \det \nabla g \tag{7}$$

in which (5) is the equation of balance of forces, (6) is a tensorial equation called the consistency relation that reflects the fact the the stress tensor in a continuum undergoing disarrangements has both an additive and a multiplicative decomposition (see the appendix in Part II of [20] and [2] for details), and (7) is a weakened version of the accommodation inequality (1). Here, $D\Psi(G)$ denotes the derivative of the response function Ψ . Because of the definition (3) of the disarrangement tensor M, the system (5) - (7) amounts to thirteen scalar relations to determine the twelve scalar fields that characterize g and G. The stress tensor S in the reference configuration is determined in the present case of purely dissipative disarrangements through the stress relation

$$S = D\Psi \tag{8}$$

and this relation then permits one to impose boundary conditions of place and/or of traction in connection with the system (5) - (7). (As in the context of classical, non-linear elasticity, the assumption that the free energy response function Ψ is frame indifferent implies that balance of angular momentum is satisfied.)

The significance of the consistency relation (6) in the present study is underscored by the following result [20] which shows that, under mild assumptions on the free energy response function Ψ , rank-one disarrangements associated with a structured deformation (g, G) that satisfies the consistency relation (6) generally decrease the free energy from its value for the corresponding (classical) structured deformation $(g, \nabla g)$.

Remark 1 Assume that the free energy response function Ψ not only is smooth

but also is rank-one convex, i.e., for all tensors A and vectors a and b such that both det A and det $(A + a \otimes b)$ are positive, there holds

$$D\Psi(A) \cdot (a \otimes b) \le \Psi(A + a \otimes b) - \Psi(A).$$
(9)

Let (g, G) a structured deformation and X a point in the body be given such that the disarrangement tensor $M(X) = \nabla g(X) - G(X)$ has rank one and such that the consistency relation (6) is satisfied. It follows that the free energy density $\Psi(G(X))$ at X for the structured deformation (g, G) is no greater than the free energy density $\Psi(\nabla g(X))$ at X for the classical deformation $(g, \nabla g)$:

$$\Psi(G(X)) \le \Psi(\nabla g(X)). \tag{10}$$

2.1 Disarrangement phases

Among the field relations (5) - (7) above, we focus attention on the consistency relation (6) that, at each point X in the body, requires that the deformation without disarrangements G(X) and the macroscopic deformation gradient $F(X) := \nabla g(X)$ satisfy

$$D\Psi(G(X))(F(X)^{T} - G(X)^{T}) = 0,$$
(11)

and on the accommodation inequality (7)

$$0 < \det G(X) \le \det F(X). \tag{12}$$

If we consider a given material point X and omit from our notation the dependence upon X, then these relations amount to the following pair of requirements

to be satisfied by tensors F and G:

$$D\Psi(G)(F^T - G^T) = 0 \quad \text{and} \quad 0 < \det G \le \det F \ . \tag{13}$$

For a given tensor F, we call a tensor G that satisfies both relations in (13) a disarrangement phase corresponding to F for the aggregate [20]. Once the tensor F is given, each disarrangement phase G corresponding to F may be thought of as a state of deformation in which the aggregate itself undergoes the homogeneous deformation $X \mapsto X_0 + F(X - X_0)$ and in which each piece undergoes the homogeneous deformation $X \longmapsto X_0 + G(X - X_0)$.

For every choice of free energy response function Ψ and for every choice of macroscopic deformation gradient F, the choice G = F satisfies both the relations in (13), and we call the resulting disarrangement phase G = F the *compact phase corresponding to* F [7]. In the compact phase, M is zero, so that there are no disarrangements, and each piece of the aggregate deforms in the same way as the aggregate itself.

For a second example of disarrangement phases, we showed [7] that, for a broad class of isotropic free energy response functions Ψ satisfying standard semiconvexity and growth properties, there exists a positive number ς_{\min} such that Ψ attains an absolute minimum at each tensor $\varsigma_{\min}R$ with R a rotation tensor. Consequently, $D\Psi(\varsigma_{\min}R) = 0$ so that for every choice of F the consistency relation (13)₁ is satisfied with $G = \varsigma_{\min}R$. In order that the the accommodation inequality (13)₂ also be satisfied for this choice of G, we must have

$$\varsigma_{\min}^3 \le \det F. \tag{14}$$

Therefore, if F satisfies (14), then for each rotation tensor R, the tensor $G = \varsigma_{\min}R$ is a disarrangement phase corresponding to F. Because $D\Psi(\varsigma_{\min}R) = 0$

each piece of the aggregate is stress-free in such a phase. Consequently, this disarrangement phase describes the aggregate in a state in which the macroscopic deformation provides via the inequality (14) enough room for each piece of the aggregate to deform into a stress-free configuration in which all the principal stretches are equal to ς_{\min} and to rotate via R. Thus, each piece of the aggregate in this phase is completely relaxed, and we call $\varsigma_{\min}R$ the loose phase corresponding to F and R.

2.2 Stable disarrangement phases

The examples available in the literature [2], [3], [7], [20] show that, given the free-energy response function Ψ and the macroscopic deformation gradient F, there are many disarrangement phases corresponding to F. The multiplicity of disarrangement phases G corresponding to a given F appearing in the different contexts suggested additional conditions for selecting preferred disarrangement phases.

In the present context of statics, an appropriate notion of stability was introduced in [20]: for a given macroscopic deformation gradient F, a tensor G is called a *stable disarrangement phase corresponding to* F if, not only is Ga disarrangement phase corresponding to F, but also G delivers the minimum energy density $\Psi(G')$ among all disarrangement phases G' corresponding to F. Thus, each stable disarrangement phase G corresponding to F is a solution to the minimization problem :

$$\min_{G'} \Psi(G') \quad \text{subject to} \quad 0 < \det G' \le \det F \quad \text{and} \quad D\Psi(G')(F^T - G'^T) = 0.$$
(15)

For example, in the context for the notion of "loose phase" described in the previous section, for each rotation R and each tensor F satisfying (14), the tensor $\varsigma_{\min}R$ is a stable disarrangement phase corresponding to F, because

 $G' = \varsigma_{\min} R$ is an absolute minimizer of the free energy response function and satisfies both relations in (15). Of course, if the tensor F does not satisfy the inequality (14), then there is no loose phase corresponding to F and R, no matter what the choice of rotation tensor R. Turning to the notion of "compact phase," we note that, while the tensor G = F always is available as the compact phase corresponding to F, this compact phase need not be a stable disarrangement phase corresponding to F, since G = F need not minimize the energy among disarrangement phases G' corresponding to F and, therefore, need not be a solution of the problem (15). Thus, for arbitrary macroscopic deformation gradients F, the compact phase corresponding to F always competes for the status of a stable disarrangement phase but need not win that status. By contrast, only for F satisfying $\varsigma_{\min}^3 \leq \det F$ is the loose phase $\varsigma_{\min}R$ a competitor; however, when it does compete, the loose phase always achieves the status of stable disarrangement phase.

Remark 1 and the notion of stable disarrangement phases corresponding to F now tell us: if the compact phase for F is a stable disarrangement phase corresponding to F, then so are all disarrangement phases G for F having F-G of rank one.

2.3 A model free energy $\Psi_{\alpha\beta}$

In order to illustrate the richness of possibilities for disarrangement phases of elastic aggregates we chose in [7] and in [20] a specific free energy response function that appears widely in the literature. We let α and β be positive numbers and consider henceforth a granular medium whose free energy response function is

$$\Psi_{\alpha\beta}(G) = \frac{1}{2}\alpha(\det G)^{-2} + \frac{1}{2}\beta tr(GG^T) = \frac{1}{2}\beta(\frac{r}{\det B_G} + trB_G)$$
(16)

where $B_G := GG^T$ is a Cauchy-Green tensor corresponding to G and $r := \alpha/\beta$. Here, the numbers α and β represent "elastic constants" for the pieces of the aggregate, and they determine the stress response in the reference configuration through the relation

$$\beta^{-1}S = \beta^{-1}D\Psi_{\alpha\beta}(G) = -\frac{r}{(\det G)^2}G^{-T} + G.$$
 (17)

It is easy to verify from the previous two relations that not only is the free energy $\Psi_{\alpha\beta}$ rank-one convex (9), but also is *strictly* rank-one convex, in the sense that equality holds in (9) if and only if a = 0 or b = 0. Rank-one convexity of $\Psi_{\alpha\beta}$ along with its smoothness imply [19] that $\Psi_{\alpha\beta}$ satisfies the Legendre-Hadamard condition: for all G with det G > 0 and for all $c, d \in \mathcal{V}$

$$D^2 \Psi_{\alpha\beta}(G) c \otimes d \cdot c \otimes d \ge 0.$$
⁽¹⁸⁾

Consequently, the lack of stability for any of the particular disarrangement phases considered in the sequel cannot be attributed to failure of the Legendre-Hadamard condition (18).

We note for this model aggregate that $D\Psi_{\alpha\beta}(G) = 0$ if and only if

$$\frac{r}{(\det G)^2}G^{-T} = G.$$

Writing $G = V_G R_G$ in its polar decomposition (with V_G symmetric and positive definite and R_G a rotation) this relation becomes $V_G^2 = r(\det V_G)^{-2}I$, with Ithe identity tensor, so that $V_G = \sqrt{r}(\det V_G)^{-1}I$. Taking the determinant of both sides tells us that $\det V_G = r^{3/8}$. Therefore, $V_G = r^{1/8}I$, and we may conclude:

$$D\Psi_{\alpha\beta}(G) = 0$$
 if and only if $G = r^{1/8}R$ for some rotation R . (19)

Thus, the only candidates for stationary points for the free energy response are $G = r^{1/8}R$ with R a rotation, and the free energy (16) at such points is given by

$$\frac{2}{\beta}\Psi_{\alpha\beta}(r^{1/8}R) = \frac{r}{r^{3/4}} + tr(r^{1/4}I) = 4r^{1/4}.$$
(20)

The growth properties of $\Psi_{\alpha\beta}$ as det G tends to zero and as $tr(GG^T)$ tends to infinity tell us that $\frac{2}{\beta}\Psi_{\alpha\beta}$ attains the absolute minimum value $4r^{1/4}$ at precisely the points $G = r^{1/8}R$ with R a rotation. From the discussion preceding (14) we conclude that for this free energy, $\zeta_{\min} = r^{1/8}$. Consequently, for each macroscopic deformation gradient F satisfying

$$r^{3/8} = \det(r^{1/8}R) \le \det F \tag{21}$$

the tensors $G = r^{1/8}R$ are the loose phases corresponding to F. In fact, for every macroscopic deformation field g that satisfies $r^{3/8} \leq \det \nabla g(X)$ for all X in the body, and for every choice of rotation field $X \mapsto Q(X)$ on the body, the structured deformation $(g, r^{1/8}Q)$ has the property that, at every point Xin the body, G(X) is a loose phase corresponding to $\nabla g(X)$. Moreover, this family of structured deformations includes all possibilities for achieving loose phases in the aggregate. The fact that the field G need not itself be a gradient tells us that the rotation field Q can vary from point to point. Therefore, the loose phases can support a texturing at the length scale of the individual pieces of the aggregate.

For each macroscopic deformation gradient F, the compact phase G = Fcorresponding to F yields the stress in the reference configuration S satisfying

$$\beta^{-1}S = F - \frac{r}{(\det F)^2}F^{-T}$$
(22)

as well as the stress in the deformed configuration T satisfying

$$\beta^{-1}(\det F)T = \beta^{-1}SF^{T} = FF^{T} - r(\det(FF^{T}))^{-1}I$$
$$= B_{F} - r(\det B_{F})^{-1}I, \qquad (23)$$

with $B_F = FF^T$.

2.4 General solutions of the consistency relation associated with $\Psi_{lphaeta}$

With a view toward determining the stable disarrangement phases of the model granular medium, we determined in [20] all of the solutions of the consistency relation $(13)_1$, which here, by (22), is equivalent to

$$(G - \frac{r}{(\det G)^2} G^{-T})(F^T - G^T) = 0.$$
(24)

Specifically, we let F be given and seek all solutions G with det G > 0 of (24), without for the moment taking into account satisfaction of the accommodation inequality (13)₂. Using again the polar decomposition $G = V_G R_G$ and the Cauchy-Green tensor $B_G = GG^T = V_G^2$, we may write (24) in the equivalent form

$$(V_G - \frac{r}{(\det V_G)^2} V_G^{-1})(R_G F^T - V_G) = 0$$

or, by multiplying the last relation on the left by V_G , in the form

$$(B_G - \frac{r}{\det B_G}I)(R_G F^T - V_G) = 0.$$
 (25)

2.4.1 The case G = F (compact phase)

We first consider the case G = F (considered above in the discussion of the compact phase corresponding to F), so that the expression $R_G F^T - V_G$ equals $R_F F^T - V_F = 0$. Consequently, the consistency relation (25) is satisfied in this case, and we have the following expressions for the Cauchy stress T = $(\det F)^{-1}D\Psi_{\alpha\beta}(G)F^T$ and for the free energy $\Psi_{\alpha\beta}(G)$:

$$\beta^{-1}(\det F)T = FF^T - \frac{r}{(\det F)^2}I$$
(26)

$$2\beta^{-1}\Psi_{\alpha\beta}(G) = \frac{r}{(\det F)^2} + tr(FF^T)$$
(27)

Of course, in this case the accommodation inequality $(13)_2$ is satisfied with equality.

2.4.2 The case $G \neq F$ (non-compact phases)

We assume now that $G \neq F$ and note from (25) that the range of $R_G F^T - V_G$ then contains non-zero elements and, hence, the nullspace of $B_G - \frac{r}{\det B_G}I$ is nontrivial. Consequently, the number $r/\det B_G$ must be one of the eigenvalues λ_1^G , λ_2^G , λ_3^G of B_G , say (without loss of generality) λ_1^G and, since $\det B_G = \lambda_1^G \lambda_2^G \lambda_3^G$, we have

$$(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r. (28)$$

At this point we invoke the Spectral Theorem to represent V_G and $B_G = V_G^2$ in terms of an orthonormal basis e_1^G , e_2^G , e_3^G of eigenvectors corresponding to the eigenvalues λ_1^G , λ_2^G , λ_3^G of B_G :

$$B_G = \sum_{i=1}^3 \lambda_i^G e_i^G \otimes e_i^G \text{ and } V_G = \sum_{i=1}^3 (\lambda_i^G)^{1/2} e_i^G \otimes e_i^G.$$
(29)

We assume without loss of generality that $e_1^G = e_2^G \times e_3^G$, and, substituting these expressions for B_G and V_G into (25), taking into account (28), and using $I = \sum_{i=1}^3 e_i^G \otimes e_i^G$ we find that the consistency relation is equivalent to to the system of vector relations

$$(\lambda_i^G - \lambda_1^G)(FR_G^T - (\lambda_i^G)^{1/2}I)e_i^G = 0 \quad \text{for} \ i = 2, 3,$$
(30)

The case $(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r$ and $\lambda_i^G \neq \lambda_1^G$ for i = 2, 3 ("plane-stress") In view of (30) we conclude in this case that the consistency relation is equivalent to the relations

$$R_G^T e_i^G = (\lambda_i^G)^{1/2} F^{-1} e_i^G \quad \text{for} \quad i = 2, 3.$$
(31)

In [20] we established the following characterization of solutions of the consistency relation (31) in the present case:

Remark 2 Let orthogonal unit vectors e and f and a linear mapping F with det F > 0 be given satisfying

$$F^{-1}e \cdot F^{-1}f = 0, \quad r^{1/2} \left| F^{-1}e \right|^3 \left| F^{-1}f \right| \neq 1, \quad r^{1/2} \left| F^{-1}e \right| \left| F^{-1}f \right|^3 \neq 1.$$
(32)

Then the tensor

$$G = r^{1/4} \left| F^{-1} e \right|^{1/2} \left| F^{-1} f \right|^{1/2} (e \times f) \otimes \left(\frac{F^{-1} e}{|F^{-1} e|} \times \frac{F^{-1} f}{|F^{-1} f|} \right) + \left| F^{-1} e \right|^{-1} e \otimes \frac{F^{-1} e}{|F^{-1} e|} + \left| F^{-1} f \right|^{-1} f \otimes \frac{F^{-1} f}{|F^{-1} f|}$$
(33)

is a solution of the consistency relation (31), and the solution (33) equals F if

and only if

$$B_F(e \times f) = \frac{r}{\det B_F} e \times f. \tag{34}$$

Moreover, every solution $G \neq F$ of the consistency relation (31) in the case $\lambda_i^G \neq \lambda_1^G$ for i = 2, 3 is of the form (33) for some choice of the orthogonal unit vectors e and f satisfying (32), and this formula for G implies that

$$V_{G} = r^{1/4} \left| F^{-1} e \right|^{1/2} \left| F^{-1} f \right|^{1/2} (e \times f) \otimes (e \times f) + \left| F^{-1} e \right|^{-1} e \otimes e + \left| F^{-1} f \right|^{-1} f \otimes f,$$
(35)

$$R_{G} = (e \times f) \otimes \left(\frac{F^{-1}e}{|F^{-1}e|} \times \frac{F^{-1}f}{|F^{-1}f|}\right) + e \otimes \frac{F^{-1}e}{|F^{-1}e|} + f \otimes \frac{F^{-1}f}{|F^{-1}f|},$$
(36)

$$\det G = r^{1/4} \left| F^{-1} e \right|^{-1/2} \left| F^{-1} f \right|^{-1/2}.$$
(37)

In addition, if $T = (\det F)^{-1} D \Psi_{\alpha\beta}(G) F^T$ is the Cauchy stress, then

$$\beta^{-1}(\det F)T = |F^{-1}e|^{-2} (1 - r^{1/2} |F^{-1}e|^3 |F^{-1}f|) e \otimes e + |F^{-1}f|^{-2} (1 - r^{1/2} |F^{-1}e| |F^{-1}f|^3) f \otimes f, \quad (38)$$

and the free energy $\Psi_{\alpha\beta}(G)$ is given by

$$\frac{2}{\beta}\Psi_{\alpha\beta}(G) = 2r^{1/2} \left| F^{-1}e \right| \left| F^{-1}f \right| + \left| F^{-1}e \right|^{-2} + \left| F^{-1}f \right|^{-2}.$$
 (39)

The formula (38) for the Cauchy stress implies that the traction $T(e \times f)$ on a plane with normal $e \times f$ is zero and that every traction vector Tn lies in the plane determined by e and f. Moreover, both Te and Tf are non-zero. It is then appropriate to use the attribute *plane-stress* to describe the solutions G in (33) of the consistency relation in the present case $\lambda_i^G \neq \lambda_1^G$ for i = 2, 3, and we use the term *plane-stress disarrangement phases corresponding to* F in referring to such tensors G that also satisfy the accommodation inequality (7) in the form $0 < \det G \leq \det F$:

$$0 < r^{1/4} \left| F^{-1} e \right|^{-1/2} \left| F^{-1} f \right|^{-1/2} \le \det F.$$
(40)

The case $(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r$ and $\lambda_2^G = \lambda_1^G$, $\lambda_3^G \neq \lambda_1^G$ ("uniaxial stress") From (30) we have in this case that the consistency relation is equivalent to the single condition

$$R_G^T e_3^G = (\lambda_3^G)^{1/2} F^{-1} e_3^G , \qquad (41)$$

and the solutions of the consistency relation in this form were characterized in [20] as follows:

Remark 3 Let a unit vector e, a proper orthogonal tensor R, and a linear mapping F with det F > 0 be given satisfying

$$R^{T}e = \frac{F^{-1}e}{|F^{-1}e|} \quad and \quad r^{1/8} |F^{-1}e| \neq 1.$$
(42)

Then the tensor G given by

$$G = r^{1/6} \left| F^{-1} e \right|^{1/3} \left(I - e \otimes e \right) R + \left| F^{-1} e \right|^{-1} e \otimes \frac{F^{-1} e}{|F^{-1} e|}$$
(43)

is a solution of the consistency relation (30) for the case $(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r$ and $\lambda_2^G = \lambda_1^G, \ \lambda_3^G \neq \lambda_1^G$. The solution G in (43) equals F if and only if $R_F = R$

and, for all vectors v perpendicular to e,

$$B_F v = \frac{r}{\det B_F} v. \tag{44}$$

Moreover, every solution of the consistency relation for this case is of the form (43) with R and e satisfying (42), and the following relations hold:

$$V_G = r^{1/6} \left| F^{-1} e \right|^{1/3} (I - e \otimes e) + \left| F^{-1} e \right|^{-1} e \otimes e \tag{45}$$

$$R_G = R \tag{46}$$

$$\det G = \det V_G = r^{1/3} \left| F^{-1} e \right|^{-1/3} \tag{47}$$

In addition, if $T = (\det F)^{-1} D \Psi_{\alpha\beta}(G) F^T$ is the Cauchy stress, then

$$\beta^{-1}(\det F)T = \frac{1 - r^{1/3} \left|F^{-1}e\right|^{8/3}}{\left|F^{-1}e\right|^2} e \otimes e,$$
(48)

and the free energy $\Psi_{\alpha\beta}(G)$ is given by

$$\frac{2}{\beta}\Psi_{\alpha\beta}(G) = 3r^{1/3} \left| F^{-1}e \right|^{2/3} + \left| F^{-1}e \right|^{-2}.$$
(49)

The formula (48) and the restriction (42) show that the state of stress in the deformed configuration of the aggregate is uniaxial and non-zero for every solution G of the consistency relation in the present case $(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r$ and $\lambda_2^G = \lambda_1^G, \ \lambda_3^G \neq \lambda_1^G$. It is then appropriate to use the attribute uniaxial stress to describe the solutions G and the term uniaxial stress disarrangement phases corresponding to F in referring to such tensors G that also satisfy the accommodation inequality (15)₂ in the form:

$$0 < r^{1/3} \left| F^{-1} e \right|^{-1/3} \le \det F.$$
(50)

The case $(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r$ and $\lambda_1^G = \lambda_2^G = \lambda_3^G$ ("zero stress"/loose phase) The relation (28) immediately yields $\lambda_1^G = \lambda_2^G = \lambda_3^G = r^{1/4}$, so that

$$B_G = r^{1/4}I$$
 and $G = r^{1/8}R$, (51)

with no restriction on the rotation $R = R_G$ imposed by the consistency relation. Of course, in this case we also have

$$\det G = r^{3/8},\tag{52}$$

and we note that this case recovers precisely those tensors G identified the previous section that render $\Psi_{\alpha\beta}$ a minimum and that enter into the description of the loose phase. We have from those considerations

$$T = 0$$
 and $2\beta^{-1}\Psi_{\alpha\beta}(G) = 4r^{1/4}$, (53)

and the accommodation inequality $(15)_2$ takes the form

$$r^{3/8} \le \det F. \tag{54}$$

2.5 The determination of stable disarrangement phases associated with $\Psi_{\alpha\beta}$ corresponding to arbitrary F

For a given macroscopic deformation tensor F, our goal is to compare the energies $\Psi_{\alpha\beta}(G)$ for the disarrangement phases G corresponding to F listed in the catalog of disarrangement phases in the previous subsection and to find the minimum energy among them. To this end one in turn may restrict $\Psi_{\alpha\beta}$ to disarrangement phases G within each of the four categories identified in the pre-

vious subsection and determine within each category all the candidates G for minima of the restriction of $\Psi_{\alpha\beta}$. Comparison among all four categories of the values $\Psi_{\alpha\beta}(G)$ so determined within each category will identify the minimum energy among all disarrangement phases. In particular, if $\Psi_{\alpha\beta}$ restricted to each category attains a minimum, one may compare the four intracategory minima to select the catalog minimum as well as the corresponding stable disarrangement phase(s) corresponding to F. For the compact phase, the intracategory minimization is trivial, because there is only one disarrangement phase in that category. For the loose phase, there may be no disarrangement phases or there may be many for the given F. In the latter case, all provide the same free energy density. Hence, the determination of intracategory minimizers for the compact and loose phases requires no effort.

Within the category "uniaxial stress", the free energy appears as a function of one unit vector e subject to the constraints provided by the accommodation inequality and the relations (42). Standard elementary methods apply readily to identify stationary values of the free energy and corresponding candidates for minimizing vectors e, and, hence candidates for stable disarragement phase G. In the "plane stress" category of disarrangement phases, the free energy is a function of two orthogonal unit vectors e and f subject to satisfaction of the accommodation inequality as well as the constraints (32). Again, standard optimization methods apply in order to identify candidates for stable disarrangement phases.

Here, we consider two simple but useful families of macroscopic deformations: (1) uniform expansions or contractions, and (2) simple shears. In the next sections we will determine for every tensor F in each family the stable disarrangement phases corresponding to F.

3 Stable disarrangement phases associated with $\Psi_{lphaeta}$ corresponding to $F=\lambda^{1/2}I$

For each positive number λ we consider the tensor $F = \lambda^{1/2}I$ representing, for $\lambda > 1$, the gradient of a uniform expansion about a given point and, for $\lambda < 1$, the gradient of a uniform contraction. The disarrangement phases listed below are obtained by substitution of $F = \lambda^{1/2}I$ into each of the categories of disarrangement phases for general F obtained earlier.

Compact disarrangement phase when $F = \lambda^{1/2} I$

$$G = \lambda^{1/2}I$$

$$\lambda^{3/2} = \lambda^{3/2} \quad (\text{accommodation inequality})$$

$$\frac{2}{\beta}\Psi_{\alpha\beta}(G) = r\lambda^{-3} + 3\lambda$$

$$\frac{1}{\beta}T = \lambda^{-1/2}(1 - r\lambda^{-4})I$$

$$M = 0$$

Plane-stress disarrangement phases when $F = \lambda^{1/2} I$

$$G = r^{1/4} \lambda^{-1/2} (e \times f) \otimes (e \times f) + \lambda^{1/2} (I - (e \times f) \otimes (e \times f))$$

$$\begin{split} r^{1/4} &\leq \lambda \quad (\text{accommodation inequality}) \\ &\frac{2}{\beta} \Psi_{\alpha\beta}(G) = 2r^{1/2}\lambda^{-1} + 2\lambda, \\ &\frac{1}{\beta}T = \lambda^{-1/2}(1 - r^{1/2}\lambda^{-2})(I - (e \times f) \otimes (e \times f)), \\ &M = \lambda^{1/2}(1 - r^{1/4}\lambda^{-1})(e \times f) \otimes (e \times f) \\ &r^{1/4} \neq \lambda. \end{split}$$

Uniaxial stress disarrangement phases when $F = \lambda^{1/2} I$

$$G = \left\{ r^{1/6} \lambda^{-1/6} I + \lambda^{1/2} \left(1 - r^{1/6} \lambda^{-2/3} \right) \ e \otimes e \right\} R$$

 $r^{1/4} \leq \lambda$ (accommodation inequality)

$$\frac{2}{\beta}\Psi_{\alpha\beta}(G) = 3r^{1/3}\lambda^{-1/3} + \lambda,$$
$$\frac{1}{\beta}T = \lambda^{-1/2}(1 - r^{1/3}\lambda^{-4/3})e \otimes e,$$
$$M = (\lambda^{1/2}I - r^{1/6}\lambda^{-1/6}R) (I - e \otimes e)$$
$$Re = e, \ r^{1/4} \neq \lambda.$$

Loose disarrangement phases when $F = \lambda^{1/2} I$

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$$G = r^{1/8}R$$

$$r^{1/4} \leq \lambda \quad (\text{accommodation inequality})$$

$$\frac{2}{\beta} \Psi_{\alpha\beta}(G) = 4r^{1/4}$$

$$T = 0$$

$$M = \lambda^{1/2}I - r^{1/8}R$$

For all but the compact phase, the accommodation inequality takes the form $r^{1/4} \leq \lambda$ and implies that the compact phase is the only competitor for stability when $\lambda < r^{1/4}$. Consequently, the compact phase $G = \lambda^{1/2} I$ is the only stable disarrangement phase corresponding to $F = \lambda^{1/2} I$ when the extension parameter λ lies in the interval $(0, r^{1/4})$. For $r^{1/4} = \lambda$ only the loose phase $G = r^{1/8}R_G$ and the compact phase G = F compete, and they yield the same value $4r^{1/4}$ of $\frac{2}{\beta}\Psi_{\alpha\beta}$. Therefore, both the loose phase $G = r^{1/8}R_G$ and the compact phase G = F are stable disarrangement phases for $F = \lambda^{1/2}I$ when $r^{1/4} = \lambda$. For λ in the interval $(r^{1/4}, \infty)$ all four categories of phases compete for stability. The relation (19) shows that, in the loose phase $G = r^{1/8}R_G$, and in the loose phase alone, $\frac{2}{\beta}\Psi_{\alpha\beta}$ attains its minimum value $4r^{1/4}$, so that only the loose phase $G = r^{1/8}R$ is a stable disarrangement phase corresponding to $F = \lambda^{1/2}I$ for λ in the interval $(r^{1/4}, \infty)$. Figure 2 shows in the $\lambda - r$ plane the stable disarrangement phases that are available corresponding to the uniform expansion/contraction $F = \lambda^{1/2}I$. While we have considered until now the ratio $r = \alpha/\beta$ as fixed, we can view the different values of r depicted in the figure as accessible via changes in the temperature (provided by the dependence of the elastic constants α and β on temperature), or accessible via replacement of a given material with response $\Psi_{\alpha\beta}$ by another with response $\Psi_{\alpha',\beta'}$ with $\alpha'/\beta' \neq \alpha/\beta$.



Figure 2: Stable disarrangement phases for $F=\lambda^{1/2}I$

We note that on the curve $\lambda = r^{1/4}$ the two stable disarrangement phases (the compact and the loose phases) not only have the same free energy density $2\beta r^{1/4} = 2\alpha^{1/4}\beta^{3/4}$ but also both have the same stress T = 0. However, when $\lambda = r^{1/4}$ and $R \neq I$, the disarrangement tensors M = 0 in the compact phase and $M = \lambda^{1/2}I - r^{1/8}R = r^{1/8}(I - R)$ in the loose phase are different, so that one cannot simply coalesce the two stable phases into one on the curve $\lambda = r^{1/4}$. For a given r > 0, when the extension parameter λ lies in the interval $(0, r^{1/4})$ in which the compact phase is stable, then the stress $T = \beta \lambda^{-1/2}(1 - r\lambda^{-4})I$ is compressive, i.e., $Tn \cdot n < 0$ for every vector n. Alternatively, when the extension parameter λ lies in the interval $(r^{1/4}, \infty)$ in which the loose phase is stable, then stress T vanishes. Consequently, for the stable disarrangement phases corresponding to $F = \lambda^{1/2}I$, the stress either is compressive or vanishes. Consequently, the stress response under uniform expansions and contractions within the stable disarrangement phases is a non-linear analogue of a "no-tension" material response [4], [5], [6].

At the present stage of our research we view the profile of stable disarrangement phases provided in Figure 2 as a statical landscape of preferred structured deformations available to the material as it expands or contracts. While it is tempting to do so, we do not at this time view the profile of stable disarrangement phases as a guide to the time evolution of changes of state as the expansion parameter λ varies with the ratio r fixed (or, alternatively, as the temperature varies with λ fixed). Further studies of the evolution of elastic aggregates in the present framework are required to determine whether or not the profile of stable disarrangement phases also provides a guide to behavior in environments that vary with time.

4 Stable disarrangement phases associated with $\Psi_{\alpha\beta}$ corresponding to $F = I + \mu a \otimes b$

In this section we consider the family of simple shears generated by fixing a pair a and b of orthogonal unit vectors that determine the plane of shearing and, for each real number μ , by taking

$$F = I + \mu a \otimes b. \tag{55}$$

We then have

$$B_F = FF^T = (I + \mu a \otimes b)(I + \mu a \otimes b)^T$$
$$= I + \mu(a \otimes b + b \otimes a) + \mu^2 a \otimes a, \tag{56}$$

whose eigenvalues are the number 1 together with largest principal stretch λ and its reciprocal:

$$\lambda : = 1 + \frac{\mu^2 + |\mu| (\mu^2 + 4)^{1/2}}{2} \ge 1,$$

$$\lambda^{-1} = 1 + \frac{\mu^2 - |\mu| (\mu^2 + 4)^{1/2}}{2} \le 1,$$
 (57)

Since the amount of shear μ can be recovered from the formula

$$\mu = \pm (\lambda + \lambda^{-1} - 2)^{1/2} = \pm \frac{|\lambda - 1|}{\lambda^{1/2}},$$

it is convenient to use the largest principal stretch $\lambda \ge 1$ to parameterize the family of simple shears. In particular, for $\lambda > 1$ the principal directions of stretch e_1^F, e_2^F , and e_3^F corresponding, respectively, to $\lambda > 1 > \lambda^{-1}$ are given by

$$e_1^F = \frac{\lambda^{1/2}}{(\lambda+1)^{1/2}}a + \frac{1}{(\lambda+1)^{1/2}}b,$$

$$e_2^F = a \times b$$

$$e_3^F = -\frac{1}{(\lambda+1)^{1/2}}a + \frac{\lambda^{1/2}}{(\lambda+1)^{1/2}}b,$$
(58)

and we restrict our attention henceforth to the non-trival case $\lambda > 1$. Consequently, we can write

$$B_F = \lambda e_1^F \otimes e_1^F + e_2^F \otimes e_2^F + \lambda^{-1} e_3^F \otimes e_3^F$$
(59)

$$\det F = \det B_F = 1, \quad trB_F = \lambda + \lambda^{-1} + 1 \tag{60}$$

$$F = V_F R_F = (\lambda^{1/2} e_1^F \otimes e_1^F + e_2^F \otimes e_2^F + \lambda^{-1/2} e_3^F \otimes e_3^F) R_F,$$
(61)

keeping in mind that e_1^F , e_2^F , and e_3^F depend upon λ according to (58). A simple computation yields expressions for V_F and R_F in terms of the original shearing vectors a and b and the principal stretch λ :

$$V_F = \frac{\lambda^2 + 1}{\lambda^{1/2}(\lambda + 1)} a \otimes a + \frac{2\lambda^{1/2}}{\lambda + 1} b \otimes b + \frac{\lambda - 1}{\lambda + 1} (a \otimes b + b \otimes a) + (a \times b) \otimes (a \times b)$$

$$(62)$$

$$R_F = \frac{2\lambda^{1/2}}{\lambda+1}(a\otimes a+b\otimes b) + \frac{\lambda-1}{\lambda+1}(a\otimes b-b\otimes a) + (a\times b)\otimes (a\times b).$$
(63)

In particular, the tensor R_F is a rotation about $a \times b$ by an angle θ_F determined by

$$\cos \theta_F = \frac{2\lambda^{1/2}}{\lambda+1}, \quad \sin \theta_F = \frac{\lambda-1}{\lambda+1}.$$
 (64)

Moreover, we have for i = 1, 2, 3:

$$B_{F}^{-1}e_{i}^{G} \cdot e_{i}^{G} = \left(\lambda^{-1}e_{1}^{F} \otimes e_{1}^{F} + e_{2}^{F} \otimes e_{2}^{F} + \lambda e_{3}^{F} \otimes e_{3}^{F}\right)e_{i}^{G} \cdot e_{i}^{G}$$
$$= \lambda^{-1}(e_{1}^{F} \cdot e_{i}^{G})^{2} + (e_{2}^{F} \cdot e_{i}^{G})^{2} + \lambda(e_{3}^{F} \cdot e_{i}^{G})^{2}, \qquad (65)$$

and this quadratic form will determine the nature of the stable disarrangement phases corresponding to simple shear.

4.1 Candidate for stability for the compact phase when $F = I + \mu a \otimes b$

For the compact phase corresponding to $F = I + \mu a \otimes b$, the results for general F in Section 2 yield the following information:

$$\begin{array}{rcl} G &=& F = I + \mu a \otimes b \\ &1 &=& 1 & (\text{Accomodation Inequality}) \\ \\ \frac{2}{\beta} \Psi_{\alpha\beta}(G) &=& r + 1 + \lambda + \lambda^{-1} \\ && \frac{1}{\beta} T &=& (\lambda - r) e_1^F \otimes e_1^F + (1 - r) e_2^F \otimes e_2^F + (\lambda^{-1} - r) e_3^F \otimes e_3^F \\ && M &=& 0 \end{array}$$

In particular, there is only one compact disarrangement phase $G = I + \mu a \otimes b$ corresponding to $F = I + \mu a \otimes b$ and, hence, only one competitor for stability for the given value of shear μ . Moreover, the compact phase arises no matter what the values of $\lambda > 1$ and r > 0, in contrast to the candidates for stability among plane-stress phases identified in the next subsection.

4.2 Candidates for stability among plane-stress disarrangement phases when $F = I + \mu a \otimes b$

The description of plane-stress disarrangement phases G for general F in Remark 2 includes the formula (39) for $\Psi_{\alpha\beta}(G)$ in the plane-stress category as well as restrictions on the vectors e and f in that formula that determine G via (43). According to our discussion of stable disarrangement phases in Section 2, we can find candidates for stable plane-stress disarrangement phases by minimizing the function

$$(e,f) \longmapsto H(e,f) = 2r^{1/2} \left| F^{-1}e \right| \left| F^{-1}f \right| + \left| F^{-1}e \right|^{-2} + \left| F^{-1}f \right|^{-2} \tag{66}$$

subject to the constraints

$$e \cdot e = f \cdot f = 1, \quad e \cdot f = 0, \quad F^{-1}e \cdot F^{-1}f = 0$$
 (67)

$$r^{1/2} \leq |F^{-1}e||F^{-1}f|$$
 (68)

$$1 \neq r^{1/2} |F^{-1}e|^3 |F^{-1}f| \tag{69}$$

$$1 \neq r^{1/2} \left| F^{-1} e \right| \left| F^{-1} f \right|^3.$$
(70)

Here, because $F = I + \mu a \otimes b$, the number det F = 1 no longer appears explicitly in the accommodation inequality (68).

The detailed steps in the solution of this minimization problem are provided in the appendix, and they permit us to compare the energies among all of the stationary plane-stress disarrangement phases G identified in that appendix. These comparisons are numerous, but elementary, and we include here only the conclusions obtained. Because different stationary phases arise in different regions of the $\lambda - r$ plane, the results of these comparisons are best viewed graphically in Figure 3. In three of the regions appearing in the figure, a formula for the minimum (normalized) energy $2\beta^{-1}\Psi_{\alpha\beta}$ for stationary planestress phases is displayed, while in the region above the line $r = \lambda$ no minimum is recorded, because no stationary, plane-stress disarrangement phases arise for this region. (The appearance twice of the minimum value $2r + 1 + r^{-1}$ is an indication that its set of competitors in the region $\lambda^{-1} < r < 1$ is different from the set of competitors in the region $1 \le r \le \lambda$.) The lack of dependence upon λ of the energy for these minima may be interpreted here as a decoupling of the energy stored in each piece of the aggregate from the amount of macroscopic shear experienced by the aggregate. It is interesting to note that, although the minimum values of energy in these plane-stress phases do not depend upon the stretch λ , other characteristics of these phases such as the stress may depend upon not only λ but also on the principal directions of stretch for G, as we shall subsequently illustrate. Employing the notation introduced at the beginning of the appendix, we note for future reference that the minimum value $2r + 1 + r^{-1}$ in the region $\lambda^{-1} < r \le \lambda$ arises from the case: r = xy and $\tau = 0$, $(\varsigma + 1)r - x^{-1} = 0$, and $(\varsigma + 1)r - r^{-1}x \neq 0$, when x = 1, while the minimum value $2r^{1/2} + 2$ for the region $0 < r \le \lambda^{-1}$ arises from the case: r < xy, $x = y = 1, \, \tau \neq 0.$

4.3 Candidates for stability among uniaxial stress disarrangement phases when $F = I + \mu a \otimes b$

The description of plane-stress disarrangement phases G for general F in Remark 3 provides among other things the formula (49) for the free energy in the uniaxial stress category along with the restrictions (42) on the rotation tensor R and the unit vector e that appear in the representation formula (43) for G. The first step in our procedure for determining stable disarrangement phases G



Figure 3: Minima of energy for plane-stress phases (simple shear).

as described in Section 2 leads us here to minimize the function J defined by

$$e \longmapsto J(e) = 3r^{1/3}(B_F^{-1}e \cdot e)^{1/3} + (B_F^{-1}e \cdot e)^{-1}$$
(71)

subject to the constraints

$$e \cdot e = 1, \quad r^2 \le B_F^{-1} e \cdot e, \quad r^{1/4} B_F^{-1} e \cdot e \ne 1.$$
 (72)

Here, we have used the fact that det F = 1 in writing the accommodation inequality in the form $(72)_2$. Because the rotation tensor R does not affect the value of the free energy, the restriction on R contained in (42) need not be considered here. In the remainder of this subsection we provide candidates for minimizers of the function J subject to the given constraints.

4.3.1 Case $r^2 = B_F^{-1} e \cdot e$

In this case, the function J can only take on the value $3r^{1/3}r^{2/3}+r^{-2}=3r+r^{-2}$, and the restriction $r^{1/4}B_F^{-1}e \cdot e \neq 1$ reduces to $r \neq 1$. The fact that e is a unit vector in the present case implies the additional inequality constraints

$$\lambda^{-1} \le r^2 \le \lambda. \tag{73}$$

4.3.2 Case $r^2 < B_F^{-1} e \cdot e$

We can find all the candidates e for minimizers of J by finding the stationary points of the function

$$e \longmapsto \Xi(e) = 3r^{1/3}(B_F^{-1}e \cdot e)^{1/3} + (B_F^{-1}e \cdot e)^{-1} + \xi(e \cdot e - 1)$$
(74)

i.e., vectors e that satisfy the constraints $(72)_{1,2,3}$, the second with strict inequality, as well as the stationarity condition

$$0 = D_e \Xi(e) = (r^{1/3} (B_F^{-1} e \cdot e)^{-2/3} - (B_F^{-1} e \cdot e)^{-2}) 2B_F^{-1} e + 2\xi e.$$

The constraint $(72)_3$ implies that the coefficient of $2B_F^{-1}e$ does not vanish, and we conclude that the stationarity condition is equivalent to the requirement that e be an eigenvector of B_F^{-1} . The three cases that then arise are listed in the table below:

e	$B_F^{-1}e \cdot e$	$r^2 < B_F^{-1} e \cdot e$	$r^{1/4}B_F^{-1}e \cdot e \neq 1$	J(e)
e_1^F	λ^{-1}	$r < \lambda^{-1/2}$	$r \neq \lambda^4$	$3r^{1/3}\lambda^{-1/3} + \lambda$
e_2^F	1	r < 1	$r \neq 1$	$3r^{1/3} + 1$
e_3^F	λ	$r < \lambda^{1/2}$	$r \neq \lambda^{-4}$	$3r^{1/3}\lambda^{1/3} + \lambda^{-1}$

At this point, we are in a position to compare the energies among all of the

stationary uniaxial stress disarrangement phases G identified above. Again, we include here only the conclusions obtained through this comparison, and we view the results graphically in Figure 4. In three of the four regions depicted in the figure, a formula for the minimum (normalized) energy $2\beta^{-1}\Psi_{\alpha\beta}$ for that region is given (within the category of uniaxial stress phases). No formula is given for the region above the curve $r = \lambda^{1/2}$, because there are no stationary phases in this category that arise in this region. (The appearance of the minimum value $1 + 3r^{1/3}$ twice indicates that its set of competitors in the region $0 < r < \lambda^{-1/2}$ is different from the set of competitors in the region $\lambda^{-1/2} \leq r < 1$.) We note for future reference that the minimum value $3r + r^{-2}$ in the region $1 \leq r \leq \lambda^{1/2}$ arises in the case $r^2 = B_F^{-1}e \cdot e$, while the minimum value $1 + 3r^{1/3}$ in the region 0 < r < 1 arises in the case $r^2 < B_F^{-1}e \cdot e$, $e = e_2^F$.



Figure 4: Minima of energy for uniaxial stress (simple shear).

4.4 Candidates for stability for the loose phases when $F = I + \mu a \otimes b$

Finally, the catalog of disarrangement phases under the category of loose phases yields the familiar formulas (with det F = 1):

$$G = r^{1/8} R_G$$
$$r \le 1$$
$$\frac{2}{\beta} \Psi_{\alpha\beta}(G) = 4r^{1/4},$$

where R_G is an arbitrary rotation. Every such disarrangement phase G corresponds to the same (global minimizing) value of the energy.

4.5 Stable disarrangement phases for simple shear

The intracategory minima for $2\beta^{-1}\Psi_{\alpha\beta}$ just obtained for the case of simple shear provide disarrangement phases for different categories that compete for the status of *stable* disarrangement phases in simple shear. From the candidates for stability obtained for the four categories in the previous subsections, we have the following regions in the quadrant $\lambda > 1, r > 0$ and intercategory competitors for stability:

- In the strip λ > 1, 0 < r < 1 the compact phase minimum r + 1 + λ + λ⁻¹, the plane-stress minimum 2r^{1/2}+2, the uniaxial stress minimum 3r^{1/3}+1, and the loose phase minimum 4r^{1/4} all compete.
- In the region λ > 1, 1 < r < λ^{1/2} the compact phase minimum r + 1 + λ + λ⁻¹, the plane-stress minimum 2r + 1 + r⁻¹, and the uniaxial stress minimum 3r + r⁻² compete.

- In the region $\lambda > 1$, $\lambda^{1/2} < r < \lambda$ the compact phase minimum $r + 1 + \lambda + \lambda^{-1}$ and the plane-stress minium $2r + 1 + r^{-1}$ compete.
- In the region $\lambda > 1, \ \lambda < r$ only the compact phase minimum $r+1+\lambda+\lambda^{-1}$ competes.

We undertake here the comparisons of the minima above in each region above, starting with the region listed last.

- For λ > 1, λ < r, only the compact phase competes, so that the compact phase corresponding to F = I + μa ⊗ b is the stable disarrangement phase in this region.
- For $\lambda > 1$, $\lambda^{1/2} < r < \lambda$, we note that the normalized energy minimum $2\beta^{-1}\Psi_{\alpha\beta}^{comp} := r+1+\lambda+\lambda^{-1}$ for the compact phase and the corresponding energy minimum $2\beta^{-1}\Psi_{\alpha\beta}^{plane} := 2r+1+r^{-1}$ for the plane-stress category of phases can be compared by comparing $\lambda + \lambda^{-1}$ and $r + r^{-1}$ on the given region. When $\lambda = r > 1$, these two expressions are equal, and, because $\frac{d}{d\lambda}(\lambda + \lambda^{-1}) = 1 \lambda^{-2} > 0$, it follows that $\lambda + \lambda^{-1} > r + r^{-1}$ for $\lambda > r$, and, therefore, $\Psi_{\alpha\beta}^{comp} > \Psi_{\alpha\beta}^{plane}$ on the given region. Because only the compact phase and the plane-stress phase compete in this region, we conclude that the plane-stress phases G that produce the normalized energy $2\beta^{-1}\Psi_{\alpha\beta}^{plane} := 2r + 1 + r^{-1}$ correspond to stable disarrangement phases for simple shear on the present region.
- For the region $\lambda > 1$, $1 < r < \lambda^{1/2}$, the argument just given shows that $\Psi_{\alpha\beta}^{comp} > \Psi_{\alpha\beta}^{plane}$ on the present region, as well, because the inequalities $1 < r < \lambda^{1/2}$ imply the inequalities $1 < r < \lambda$ employed in the previous region. The comparison of $2\beta^{-1}\Psi_{\alpha\beta}^{uniax} := 3r + r^{-2}$ and $2\beta^{-1}\Psi_{\alpha\beta}^{plane} = 2r + 1 + r^{-1}$ amounts to comparing $r + r^{-2}$ and $1 + r^{-1}$, and it is easy to show that, for r > 1, $r + r^{-2} > 1 + r^{-1}$, so that $\Psi_{\alpha\beta}^{uniax} > \Psi_{\alpha\beta}^{plane}$ on the

present region. (Actually, an elementary argument allows us to conclude that

$$\Psi_{\alpha\beta}^{comp} > \Psi_{\alpha\beta}^{uniax} > \Psi_{\alpha\beta}^{plane}$$

on this region.) Therefore, the plane-stress disarrangement phases G that produce the normalized energy $2\beta^{-1}\Psi^{plane}_{\alpha\beta} := 2r+1+r^{-1}$ also corresponds to a stable disarrangement phase for simple shear on the region $\lambda > 1$, $1 < r < \lambda^{1/2}$.

• For $\lambda > 1, 0 < r < 1$ we repeatedly use the arithmetic-geometric mean inequality

$$p_1 + \dots + p_k \ge k(p_1 \cdots p_k)^{1/k}$$

for various values of the positive integer k and the positive numbers p_1, \ldots, p_k to conclude that

$$\begin{aligned} r+1+\lambda+\lambda^{-1} &\geq & 2r^{1/2}+2 \\ &= & r^{1/2}+r^{1/2}+1+1 \geq 3r^{1/3}+1 \\ &= & r^{1/3}+r^{1/3}+r^{1/3}+1 \geq 4r^{1/4}, \end{aligned}$$

and, therefore, that on $\lambda > 1, 0 < r < 1$ there holds

$$\Psi_{\alpha\beta}^{comp} > \Psi_{\alpha\beta}^{plane} > \Psi_{\alpha\beta}^{uniax} > \Psi_{\alpha\beta}^{loose}.$$

Consequently, loose disarrangement phases provide stable disarrangement phases in simple shear in this region.

The arguments above show that, for simple shear, in the only region $\lambda > 1, 0 < r < 1$ where loose disarrangement phases can compete, they are necessarily stable, in agreement with the general conclusion drawn in Section 2. Our

arguments also show that the compact phase competes in all cases, again in agreement with Section 2. However, for simple shear, we can conclude from above that the compact phase in every region provides the largest energy among the competing phases and that the only region where the compact phase is a stable disarrangement phase is the one in which it is the sole competitor for stability. The stable phases for simple shear that we have determined above as well as their regions of stability are depicted in Figure 5. The tables below



Figure 5: Stable phases for simple shear.

display these stable disarrangement phases for $F = I + \mu a \otimes b$, including information tabulated earlier for all disarrangement phases and refined here through our subsequent analysis. As in (57), we have $\lambda = 1 + \frac{\mu^2 + |\mu|(\mu^2 + 4)^{1/2}}{2}$; moreover, the principal directions for F are given by (58), and the principal directions for G in the plane-stress category are restricted as indicated:

Category	Stable phase(s) G	Principal directions of G
Compact	F	$e^F_i,i=1,2,3$
Plane-stress	(75)	$e = \pm e_2^F, f = \cos \theta e_1^F + \sin \theta e_3^F, \pm e_2^F \times f$
Loose	$r^{1/8}R$	all directions

Category	Stability region	Energy $2\beta^{-1}\Psi_{\alpha\beta}$	Stress $\beta^{-1}T$
Compact	$1 < \lambda, \ \lambda < r$	$r+1+\lambda+\lambda^{-1}$	$FF^T - rI$
Plane-stress	$1 < \lambda, \ 1 < r < \lambda$	$2r + 1 + r^{-1}$	$(1-r)e\otimes e + (r^{-1}-r)f\otimes f$
Loose	$\lambda \geq 1, \ 0 < r < 1$	$4r^{1/4}$	0

The entry "Stable phase(s) G" for the plane-stress category is the following expression:

$$G = r^{1/2}(e \times f) \otimes \left(\frac{F^{-1}e}{|F^{-1}e|} \times \frac{F^{-1}f}{|F^{-1}f|}\right) + e \otimes \frac{F^{-1}e}{|F^{-1}e|} + r^{-1/2}f \otimes \frac{F^{-1}f}{|F^{-1}f|},$$
(75)

and, in the entry "Principal directions of G" for the plane-stress category, the angle θ is restricted through the relation

$$\cos^2 \theta = \frac{\lambda(\lambda - r)}{\lambda^2 - 1}.$$
(76)

The information in Figure 5 and in the tables provides a landscape of the stable disarrangement phases available in simple shear. In the compact phase, because G = F, the deformation without disarrangement G that identifies the phase is completely specified once F is given. In the loose phases, G is the scalar $r^{1/8}$ multiplied by an arbitrary rotation R. In the plane-stress phase, , the stable disarrangement phase G is completely determined by the four vectors $e, f, F^{-1}e$, and $F^{-1}f$, with e and f given in the table. Consequently, apart from a choice of

sign for e and choices of signs in solving the relations $\cos^2 \theta = \frac{\lambda(\lambda - r)}{\lambda^2 - 1}$ for $\cos \theta$ and $\sin^2 \theta = \frac{\lambda r - 1}{\lambda^2 - 1}$ for $\sin \theta$, the stable plane-stress phase G is completely determined by $F = I + \mu a \otimes b$. The rotation R_G corresponding to this stable disarrangement phase is given in Remark 2, and the principal stretches of $B_G = GG^T$ are $\lambda_1^G = r$, $\lambda_2^G = 1$, and $\lambda_3^G = r^{-1}$.

In the compact phase, the Cauchy stress T has principal stresses $\beta(\lambda - r)$, $\beta(1-r),\,\beta(\lambda^{-1}-r)$, so that, in the region of stability for the compact phase, the principal stresses are all negative and vary with the stretch λ . In the stable, plane stress phase, the formula in the table gives the Cauchy stress T as a linear combination of the dyads $e \otimes e$ and $f \otimes f$ in which only the dyad $f \otimes f$ varies with the stretch λ . The principal stresses for this stable disarrangement phase are 0, $\beta(1-r)$ and $\beta(r^{-1}-r)$, the latter two of which are negative in the region of stability for this disarrangement phase and do not vary with λ . In the loose phase, the stress vanishes as do all the principal stresses. Thus, for all of the stable disarrangement phases, the non-zero principal stresses are negative in the region of stability. In the two regions where the compact phase is not a stable disarrangement phase, the stable phase is such that one principal stress vanishes or all three principal stresses vanish, and all of the principal stresses are independent of the stretch λ . We conclude that the requirement of stability for a disarrangement phase in the case of simple shear entails all of the pieces of the aggregate to be subject to no tensile tractions, i.e., $Tn \cdot n \leq 0$ for all unit vectors n, and stability for the compact disarrangement phase is characterized by the condition: $Tn \cdot n < 0$ for all unit vectors n. Consequently, the stable disarrangement phases in simple shear for an aggregate with the energy $\Psi_{\alpha\beta}$ display the characteristics of a "no-tension or masonry-like material with nonlinear elastic response" (see [4], [5], [6] for studies of no-tension/masonry-like materials with linear elastic response).

4.6 Shapes and orientations of deformed pieces of the aggregate in stable phases for simple shear

We recall that for every structured deformation, the Approximation Theorem permits us to identify the deformation without disarrangements G as the contribution at the macrolevel of submacroscopic deformations without disarrangements. A form of this identification relation that is useful here is the formula (see [1]):

$$G(X) = \lim_{\varepsilon \to 0} \lim_{n \to \infty} \frac{\int_{B(X,\varepsilon)} \nabla f_n(Y) dV_Y}{volB(X,\varepsilon)}$$

We can think of the size of the pieces of the aggregate going to zero as the index n tends to infinity, so that, in the context of aggregates, G(X) represents the average deformation $\frac{\int_{B(X,\varepsilon)} \nabla f_n(Y) dV_Y}{vol B(X,\varepsilon)}$ of pieces of the aggregate within a ball of radius ε , computed in the limit as the size of the pieces tends to zero and, subsequently, as ε tends to zero.

We describe here the geometry of the deformed pieces of the aggregate in terms of the principal stretches of G for each stable disarrangement phase in simple shear. The following table displays these principal stretches along with their effect on a unit sphere:

Stable phase	Principal stretches of G	Image of unit sphere under G
Compact	$\lambda^{1/2}, 1, \lambda^{-1/2}$	ellipsoid; shape depends on λ
Plane-stress $r^{1/2}, 1, r^{-1/2}$		ellipsoid; shape independent of λ
Loose	$r^{1/8}, r^{1/8}, r^{1/8}$	sphere; size independent of λ

The table shows that the only stable phase in which the shape of deformed pieces of the aggregate depends upon the macroshear λ is the compact phase. Of course, in this phase G = F, and we cannot distinguish the geometrical changes in the pieces of the aggregate from those in the aggregate, itself. In the loose phases of the aggregate, the deformation without disarrangement G causes changes in the pieces of the aggregate that, on average, take the unit sphere into a sphere of radius $r^{1/8}$, independent of the macroshear λ . All vectors are principal directions of G for these loose phases, so that the principal directions also are independent of λ . By contrast, in each stable, plane-stress phase the deformation of the pieces of the aggregate, on average, takes the unit sphere into an ellipsoid with semiaxes of length $r^{1/2}$, 1, $r^{-1/2}$. The amount of macroshear λ of the aggregate does not influence the deformed shape of the pieces.

From the results obtained in the appendix, we must keep in mind that the principal directions f and $e \times f$ of G in the stable plane-stress phase do depend in a non-trivial way on the macroshear through the principal directions

$$e_3^G = f = \cos \theta e_1^F + \sin \theta e_3^F, \text{ with } \theta \text{ satisfying (76)}$$
$$e_1^G = \pm e_2^F \times f = \pm (\sin \theta e_1^F - \cos \theta e_3^F). \tag{77}$$

When $\lambda = r$ the relation (76) yields $\cos^2 \theta = 0$, and we obtain

$$\begin{array}{ll} e^G_3 & \mid & _{\lambda=r}=\pm e^F_3 \\ e^G_1 & \mid & _{\lambda=r}=\pm e^F_1 \end{array}$$

and we conclude that the principal directions of F and of G coincide when $\lambda = r$. As $\lambda \mapsto \infty$ the relation (76) yields $\cos^2 \theta \longrightarrow 1$, and we obtain

$$\begin{array}{ll} e_3^G & \mid & \lambda {\longrightarrow} \infty = \pm e_1^F \\ e_1^G & \mid & \lambda {\longrightarrow} \infty = \mp e_3^F \end{array}$$

and this tells us that, in the limit as the stretch λ tends to ∞ , the principal

directions of G in the plane of shearing are again principal directions of F, but corresponding to different amounts of stretch. These results tell us that the orientations of the deformed pieces of the aggregate as they appear in the stable, plane-stress phase when $\lambda = r$ are the same as the orientation of the principal directions of the simple shear F. For values of stretch λ greater than r the orientation of the deformed pieces in the plane of shearing is rotated with respect to the principal directions of F by an angle that tends to $\pm \pi/2$ as the stretch increases without bound. In otherwords, while the shapes of the pieces of the aggregate do not vary with the macrostretch λ , their orientations relative to the principal directions of F in the stable plane-stress phase for large macroshears λ are rotated in the plane of shearing by an amount that tends to $\pm \pi/2$ (see Figure 6).



Figure 6: Relative orientation of principal axis of G and F.

5 Appendix: Details of the analysis of planestress disarrangement phases when $F = I + \mu a \otimes b$

We devote this appendix to the details of the analysis of the minimization problem (66) - (70) which we restate here for convenience: minimize the function

$$(e,f) \longmapsto H(e,f) = 2r^{1/2} \left| F^{-1}e \right| \left| F^{-1}f \right| + \left| F^{-1}e \right|^{-2} + \left| F^{-1}f \right|^{-2}$$
(78)

subject to the constraints

$$e \cdot e = f \cdot f = 1, \quad e \cdot f = 0, \quad F^{-1}e \cdot F^{-1}f = 0$$
 (79)

$$r^{1/2} \leq |F^{-1}e||F^{-1}f|$$
 (80)

$$1 \neq r^{1/2} |F^{-1}e|^3 |F^{-1}f|$$
(81)

$$1 \neq r^{1/2} |F^{-1}e| |F^{-1}f|^3.$$
(82)

If we ignore for the moment the last two constraints, (81) and (82), then the set of pairs (e, f) satisfying the remaining constraints forms a closed, bounded subset of $\mathcal{V} \times \mathcal{V}$. If this set is not empty, i.e., if the constraints (79) and (80) admit at least one pair (e, f), we may conclude that the continuous function $(e, f) \mapsto H(e, f)$ in (78) attains a minimum on that set. Of course, we must check a posteriori that such a minimum complies with the last two constraints (81) and (82). It is convenient in solving this constrained minimization problem to use the notation and identities

$$x := B_F^{-1} e \cdot e = \left| F^{-1} e \right|^2, \quad y := B_F^{-1} f \cdot f = \left| F^{-1} f \right|^2$$
(83)

$$F^{-1}e \cdot F^{-1}f = B_F^{-1}e \cdot f = e \cdot B_F^{-1}f$$
(84)

which allow us to write the partial derivatives $D_e H(e, f)$ and $D_f H(e, f)$ in the concise forms

$$D_e H(e, f) = 2(r^{1/2}x^{3/2}y^{1/2} - 1)x^{-2}B_F^{-1}e$$

$$D_f H(e, f) = 2(r^{1/2}y^{3/2}x^{1/2} - 1)y^{-2}B_F^{-1}f.$$
 (85)

According to the constraints (81) and (82), the coefficients of the vectors $B_F^{-1}e$ and $B_F^{-1}f$ on the right-hand sides of (85) are non-zero and, therefore, the partial derivatives, themselves, are non-zero vectors.

5.1 Case:
$$r^{1/2} < |F^{-1}e| |F^{-1}f| \iff r < xy$$

In view of (83) the accommodation inequality (80) may be written in this case as $r \leq xy$, and, in seeking candidates for minimizers of H in (78), we may first impose this constraint on e and f as the strict inequality

$$r < xy. \tag{86}$$

Consequently, for this case we may limit the constraints on e and f to the four scalar constraints contained in the relations (79). For $F = I + \mu a \otimes b$ and $\mu \neq 0$ (or, equivalently, $\lambda > 1$), these constraints are independent, and we therefore may use the method of Lagrange multipliers to identify stationary points of the function H restricted to the constraint set defined by (79). Accordingly, we seek stationary points of the function Φ on $\mathcal{V} \times \mathcal{V}$ defined by

$$\Phi(e,f) = H(e,f) + \xi(e \cdot e - 1) + \eta(f \cdot f - 1) + 2\sigma e \cdot f + 2\tau B_F^{-1} e \cdot f, \quad (87)$$

i.e., we seek vectors e and f as well as scalars ξ , η , σ , and τ such that not only are the constraints (79) but also the stationarity conditions

$$D_e \Phi(e, f) = D_f \Phi(e, f) = 0 \tag{88}$$

are satisfied. Differentiation of (87) and use of the formulas (85) as well as the constraints (79) yield

$$(r^{1/2}x^{3/2}y^{1/2} - 1)x^{-2}B_F^{-1}e + \tau B_F^{-1}f = (r^{1/2}x^{3/2}y^{1/2} - 1)x^{-1}e - \sigma f$$

$$\tau B_F^{-1} e + (r^{1/2} x^{1/2} y^{3/2} - 1) y^{-2} B_F^{-1} f = -\sigma e + (r^{1/2} x^{1/2} y^{3/2} - 1) y^{-1} f$$

$$\sigma = -\tau x = -\tau y, \qquad (89)$$

and, in particular, there holds: $\tau(x - y) = 0$. There arise also formulas for the multipliers ξ and η in terms of x, y, and r that we need not record here.

5.1.1 Case: $r^{1/2} < \left|F^{-1}e\right| \left|F^{-1}f\right|$ and $\tau = 0$.

As we observed above, $r^{1/2}x^{3/2}y^{1/2} - 1 \neq 0$ and $r^{1/2}x^{1/2}y^{3/2} - 1 \neq 0$, and the condition $\tau = 0$ along with (89) yield the simple relations:

$$B_F^{-1}e = xe \quad \text{and} \quad B_F^{-1}f = yf.$$
(90)

Hence, the only candidates (e, f) for stationarity of Φ here are orthogonal pairs of unit eigenvectors of B_F^{-1} , all of which are generated from the following table

e	f	x	y	xy > r	$rx^3y \neq 1$	$rxy^3 \neq 1$	H(e,f)
e_1^F	e_2^F	λ^{-1}	1	$r^{-1} > \lambda$	$r \neq \lambda^3$	$r\neq \lambda$	$2r^{1/2}\lambda^{-1/2} + 1 + \lambda$
e_1^F	e_3^F	λ^{-1}	λ	1 > r	$r \neq \lambda^2$	$r \neq \lambda^{-2}$	$2r^{1/2} + \lambda^{-1} + \lambda$
e_2^F	e_3^F	1	λ	$\lambda > r$	$r \neq \lambda^{-1}$	$r \neq \lambda^{-3}$	$2r^{1/2}\lambda^{1/2} + 1 + \lambda^{-1}$
							(91

(using symmetries in H to obtain all possibilities from those in the table):

We note that the constraint $(79)_4$ is satisfied in all of these cases, because e and f are orthogonal.

5.1.2 Case: $r^{1/2} < \left|F^{-1}e\right| \left|F^{-1}f\right|$ and $\tau \neq 0$.

Because $\tau(x-y) = 0$ and $\tau \neq 0$, we have in this case x = y, which implies $r < x^2$, and some straightforward calculations show that the relations (89) reduce to

$$\left(\tau - \frac{(r^{1/2}x^2 - 1)^2}{\tau x^2}\right) (B_F^{-1}e - xe) = 0$$

$$\left(\tau - \frac{(r^{1/2}x^2 - 1)^2}{\tau x^2}\right) (B_F^{-1}f - xf) = 0.$$
(92)

We observe that the scalar factor that appears on the left-hand side of both of these relations must be zero. Otherwise, both e and f would be eigenvectors of B_F^{-1} corresponding to the same eigenvalue x. Because e and f are orthogonal and the eigenspaces of B_F^{-1} for a simple shear are one-dimensional, this cannot occur. Consequently, we have in the present case

$$\tau^2 = \frac{(r^{1/2}x^2 - 1)^2}{x^2},\tag{93}$$

and we note that this formula is consistent with the case requirement $\tau \neq 0$ by virtue of (81). Thus, the present case requires that at most one of e and f are eigenvectors of B_F^{-1} .

We first consider the case where exactly one of e and f is an eigenvector of B_F^{-1} . Since $B_F^{-1}e \cdot e = x = y = B_F^{-1}f \cdot f$, the only possible eigenvalue of B_F^{-1} that can arise corresponding to e or f is the intermediate eigenvalue 1 with eigenvector $\pm e_2^F$. For definiteness, if $B_F^{-1}e = e$, then x = 1 = y and

$$e = \pm e_2^F$$
 and $f = X e_1^F + Z e_3^F$ with $XZ \neq 0.$ (94)

Moreover, since f is a unit vector and $B_F^{-1}e \cdot e = 1 = B_F^{-1}f \cdot f$, we have

$$X^{2} + Z^{2} = 1$$
 and $\lambda^{-1}X^{2} + \lambda Z^{2} = 1$, (95)

and these relations tell us that $X = \pm (\frac{\lambda}{\lambda+1})^{1/2}$ and $Z = \pm (\frac{1}{\lambda+1})^{1/2}$, with all four combinations of sign choices permissible. Thus, in the present case, if $e = \pm e_2^F$, then $f = \pm (\frac{\lambda}{\lambda+1})^{1/2} e_1^F \pm (\frac{1}{\lambda+1})^{1/2} e_3^F$, and we have

$$H(e,f) = 2r^{1/2} + 2.$$
(96)

The relations (81) and (82) in this case both reduce to $r \neq 1$, and the accommodation inequality becomes r < 1.

We consider now the alternative case where neither e nor f is an eigenvector of B_F^{-1} . Because $B_F^{-1}e \cdot f = e \cdot f = 0$ and $B_F^{-1}e \times e \neq 0$, the unit vector f is given by

$$f = \frac{B_F^{-1}e \times e}{\left|B_F^{-1}e \times e\right|},\tag{97}$$

so that we may use this formula to compute $B_F^{-1}f \cdot f$ in terms of $B_F^{-1}e$, B_Fe , and e as follows. First we note from (97) that

$$B_{F}^{-1}f \cdot f = \frac{B_{F}^{-1}(B_{F}^{-1}e \times e)}{|B_{F}^{-1}e \times e|} \cdot \frac{B_{F}^{-1}e \times e}{|B_{F}^{-1}e \times e|}$$
$$= |B_{F}^{-1}e \times e|^{-2} B_{F}^{-1}(B_{F}^{-1}e \times e) \cdot (B_{F}^{-1}e \times e).$$
(98)

 B_F^{-1} is symmetric with determinant 1, and we may write

$$B_F^{-1}(B_F^{-1}e \times e) = (B_F B_F^{-1})e \times B_F e = e \times B_F e.$$

Consequently, $B_F^{-1}(B_F^{-1}e \times e) \cdot (B_F^{-1}e \times e)$ is of the form

$$(u \times v) \cdot (w \times z) = (u \cdot w)(v \cdot z) - (u \cdot z)(w \cdot v),$$

with u = e, $v = B_F e$, $w = B_F^{-1} e$, and z = e, and, recalling that $x = B_F^{-1} e \cdot e$, we have

$$B_F^{-1}(B_F^{-1}e \times e) \cdot (B_F^{-1}e \times e) = (e \cdot B_F^{-1}e)(B_F e \cdot e) - (e \cdot e)(B_F^{-1}e \cdot B_F e)$$

= $x(B_F e \cdot e) - 1$ (99)

We also have

$$|B_F^{-1}e \times e|^{-2} = (|B_F^{-1}e \times e|^2)^{-1}$$

= $(|B_F^{-1}e|^2 |e|^2 - (B_F^{-1}e \cdot e)^2)^{-1}$
= $(|B_F^{-1}e|^2 - x^2)^{-1}$ (100)

and, by (98), (99), and (100) we conclude that

$$x = y = B_F^{-1} f \cdot f$$

= $\frac{x(B_F e \cdot e) - 1}{|B_F^{-1}e|^2 - x^2}.$

We have thus shown that $x=B_F^{-1}e\cdot e~$ is a root of the cubic equation

$$x^{3} + (B_{F} e \cdot e - \left|B_{F}^{-1} e\right|^{2})x - 1 = 0.$$
(101)

Writing $e = Xe_1^F + Ye_2^F + Ze_3^F$ with $X^2 + Y^2 + Z^2 = 1$, we note that

$$x = B_F^{-1} e \cdot e = \lambda^{-1} X^2 + Y^2 + \lambda Z^2$$

= 1 + (\lambda - 1)(Z^2 - \lambda^{-1} X^2), (102)

$$B_F e \cdot e = \lambda X^2 + Y^2 + \lambda^{-1} Z^2$$

= 1 + (\lambda - 1)(X^2 - \lambda^{-1} Z^2), (103)

$$|B_F^{-1}e|^2 = (\lambda^{-1}X)^2 + Y^2 + (\lambda Z)^2$$

= 1 + (\lambda^2 - 1)(Z^2 - \lambda^{-2}X^2), (104)

and a short calculation using (102) - (104) shows that the coefficient of x in (101) is given by

$$B_F e \cdot e - \left| B_F^{-1} e \right|^2 = \lambda^{-1} (\lambda^3 - 1) (\lambda^{-1} X^2 - Z^2) = (\lambda + 1 + \lambda^{-1}) (1 - x).$$

Consequently, the cubic equation for x becomes

$$0 = x^{3} - (\lambda + 1 + \lambda^{-1})x^{2} + (\lambda + 1 + \lambda^{-1})x - 1$$
$$= (x - 1)(x - \lambda)(x - \lambda^{-1}).$$

The roots $x = B_F^{-1}e \cdot e = \lambda$ and $x = B_F^{-1}e \cdot e = \lambda^{-1}$ are ruled out, for then e would be an eigenvector of B_F^{-1} , contradicting the specification of the present case. We conclude that x = y = 1, so that e and f must be perpendicular vectors that are not eigenvectors of B_F^{-1} and that both lie on the intersection of the unit sphere $\{v \in \mathcal{V} \mid v \cdot v = 1\}$ and the ellipsoid $\{v \in \mathcal{V} \mid B_F^{-1}v \cdot v = 1\}$. Because x = y = 1, the condition that e and f not be eigenvectors of B_F^{-1} then is equivalent to the conditons $e \neq \pm e_2^F$ and $f \neq \pm e_2^F.$

In summary, the case $r^{1/2} < |F^{-1}e| |F^{-1}f|$ and $\tau \neq 0 \implies r < x^2$, with neither e nor f eigenvectors of B_F^{-1} , necessitates that $x = y = B_F^{-1}e \cdot e = B_F^{-1}f \cdot f = 1$ and, by (102), that

$$e = Xe_1^F + Ye_2^F + Ze_3^F$$
 with $X^2 = \lambda Z^2$ and $X^2 + Y^2 + Z^2 = 1.$ (105)

Moreover, the formula (97) then determines the vector f in terms of B_F^{-1} and e. It remains to show that these necessary conditions on e and on f for stationarity of H actually can be satisfied. To this end, we use (105) to conclude that

$$e = \sigma_1 \lambda^{1/2} Z e_1^F + \sigma_2 (1 - (1 + \lambda) Z^2)^{1/2} e_2^F + Z e_3^F$$
(106)

with $|\sigma_1| = |\sigma_2| = 1$ and with

$$0 < |Z| < (1+\lambda)^{-1/2}, \tag{107}$$

and the relation (97) then yields the formula

$$f = \frac{Z}{|Z|(\lambda+1)^{1/2}} \left\{ \sigma_2 \lambda^{1/2} (1 - (1+\lambda)Z^2)^{1/2} e_1^F - \sigma_1 (\lambda+1) Z e_2^F + \sigma_1 \sigma_2 (1 - (1+\lambda)Z^2)^{1/2} e_3^F \right\}.$$
(108)

It can easily be verified that the vectors e and f in (106) and (108) satisfy the constraints (79) - (82), provided that r < 1. The free energy H(e, f) is given again by the formula (96).

5.2 Case:
$$r^{1/2} = |F^{-1}e| |F^{-1}f| \iff r = xy$$

We treat the relation r = xy that defines the present case as a constraint to be appended to the previous ones (79) - (82), and, accordingly, we seek stationary pairs (e, f) for the function Π defined by

$$\Pi(e, f) := \Phi(e, f) + \varsigma \left((B_F^{-1}e \cdot e)(B_F^{-1}f \cdot f) - r \right)$$

= $H(e, f) + \xi(e \cdot e - 1) + \eta \left(f \cdot f - 1 \right) + 2\sigma e \cdot f + 2\tau B_F^{-1}e \cdot f + \varsigma \left((B_F^{-1}e \cdot e)(B_F^{-1}f \cdot f) - r \right),$ (109)

with H the energy defined in (78). The constraints and the condition that the derivatives of Π vanish yield the relations

$$\begin{aligned} ((\varsigma+1)rx-1)x^{-2}B_F^{-1}e + \tau B_F^{-1}f &= ((\varsigma+1)r - x^{-1})e - \sigma f \\ \tau B_F^{-1}e + ((\varsigma+1)x - r^{-2}x^2)B_F^{-1}f &= -\sigma e + ((\varsigma+1)r - r^{-1}x)f \\ \sigma &= -\tau x = -\tau y = -\tau r x^{-1}. \end{aligned}$$
(110)

(The multipliers ξ and η were expressed in terms of r, x, and ζ and then were eliminated from further consideration in the course of deriving these relations.)

5.2.1 Case: r = xy and $\tau \neq 0$.

For this case the equation $(110)_3$ tells us that $x = y = r^{1/2}$, and elementary but lengthy algebraic manipulations show that there is no value of r that makes $x = y = r^{1/2}$ consistent with the full set of constraints (79) - (82). Consequently, the case r = xy and $\tau \neq 0$ cannot occur.

5.2.2 Case: r = xy and $\tau = 0$.

The stationarity conditions (110) with $\tau = 0$ tell us that $\sigma = 0$, and multiplication of the first by x^2 and the second by r/x yields

$$((\varsigma+1)r - x^{-1})(B_F^{-1}e - xe) = 0$$

$$((\varsigma+1)r - r^{-1}x)(B_F^{-1}f - rx^{-1}f) = 0.$$
 (111)

We analyze these stationarity conditions according to whether or not each of the two scalar coefficients $(\varsigma + 1)r - x^{-1}$ and $(\varsigma + 1)r - r^{-1}x$ appearing in the left-hand members vanishes.

Case: r = xy and $\tau = 0$ and $(\varsigma + 1)r - x^{-1} = (\varsigma + 1)r - r^{-1}x = 0$ Here we conclude that $x = r^{1/2} = rx^{-1} = y$, and, as stated in the case: r = xy and $\tau \neq 0$, these relations are not consistent with the full set of constraints.

Case: r = xy and $\tau = 0$ and $((\varsigma + 1)r - x^{-1})((\varsigma + 1)r - r^{-1}x) \neq 0$ For this case, both of the coefficients appearing in (111) are non-zero, and we conclude that e and f are eigenvectors of B_F^{-1} corresponding to eigenvalues x and rx^{-1} , respectively. Because F is a simple shear and $e \cdot f = 0$, the two eigenvalues must be distinct, $x \neq rx^{-1}$, and only the following three possibilities can occur (omitting duplications due to the symmetry of the present conditions with respect to e and f and with respect to x and y):

x	e	$y = rx^{-1}$	f	H(e,f)	$rx^3y \neq 1, rxy^3 \neq 1$
1	e_2^F	$\lambda = r$	e_3^F	$2\lambda+1+\lambda^{-1}$	$r \neq 1$
1	e_2^F	$\lambda^{-1} = r$	e_1^F	$2\lambda^{-1} + 1 + \lambda$	$r \neq 1$
λ	e_3^F	$\lambda^{-1} = r \lambda^{-1}$	e_1^F	$2+\lambda^{-1}+\lambda$	$1=r\neq\lambda^{-2}, 1=r\neq\lambda^2$

The disarrangement phases G given via (33) for each of the three possibilities in this table are candidates for stable disarrangement phases in simple shear.

Case: r = xy and $\tau = 0$, $(\varsigma + 1)r - x^{-1} = 0$, and $(\varsigma + 1)r - r^{-1}x \neq 0$. In this case, $x^{-1} \neq r^{-1}x$ which is equivalent to $y = x^{-1}r \neq x$. By (111), $B_F^{-1}e = xe$, and, therefore, $x \in \{\lambda, 1, \lambda^{-1}\}$. We consider in detail the case x = 1 for which, necessarily, $e = \pm e_2^F$, and we carry out the analysis for $e = +e_2^F$. Because $e \cdot f = 0$, there is a number $\theta \in [0, 2\pi)$ such that $f = \cos \theta e_1^F + \sin \theta e_3^F$, and we have not only $B_F^{-1}e \cdot f = 0$, but also

$$r = rx^{-1} = y = B_F^{-1}f \cdot f = \lambda^{-1}\cos^2\theta + \lambda(1 - \cos^2\theta)$$

which yields the formula

$$\cos^2 \theta = \frac{\lambda(\lambda - r)}{\lambda^2 - 1}.$$
(112)

Since $0 \le \cos^2 \theta \le 1$ and $1 < \lambda$, the fraction on the right-hand side of (112) lies in the closed interval [0, 1], and we conclude that

$$\lambda \ge r \quad \text{and} \quad \lambda \ge r^{-1}.$$
 (113)

Because x = 1 and y = r, the formula (78) tells us that $H(e, f) = 2r + 1 + r^{-1}$. In the present case the restrictions $rx^3y \neq 1$, $rxy^3 \neq 1$ both become $r \neq 1$.

The case $x = \lambda$ and the case $x = \lambda^{-1}$ are treated in a similar manner, and we collect the conclusions in the three cases in the following tables:

x	e	y	f	H(e,f)
1	$\pm e_2^F$	r	$\cos \theta e_1^F + \sin \theta e_3^F, \cos^2 \theta = \frac{\lambda(\lambda - r)}{\lambda^2 - 1}$	$2r + 1 + r^{-1}$
λ^{-1}	$\pm e_1^F$	λr	$\cos\theta e_2^F + \sin\theta e_3^F, \cos^2\theta = \frac{\lambda(1-r)}{\lambda-1}$	$2r + \lambda + \lambda^{-1}r^{-1}$
λ	$\pm e_3^F$	$r\lambda^{-1}$	$\cos\theta e_1^F + \sin\theta e_2^F, \cos^2\theta = \frac{\lambda - r}{\lambda - 1}$	$2r + \lambda^{-1} + \lambda r^{-1}$

x	Constraints
1	$r \neq 1, \lambda \geq r, \lambda \geq r^{-1}$
λ^{-1}	$r \le 1, r^{-1} \le \lambda, r \ne \lambda^{-1/2}, r \ne \lambda^{-1}$
λ	$1 \le r \le \lambda, r \ne \lambda^{-1/2}, r \ne \lambda^{-2}$

The disarrangement phases G given via (33) for each of the three possibilities in this table are also candidates for stable disarrangement phases in simple shear.

Case: r = xy and $\tau = 0$, $(\varsigma + 1)r - x^{-1} \neq 0$, and $(\varsigma + 1)r - r^{-1}x) = 0$. This case amounts to interchanging the roles of x and of y and, consequently, those of e and f in the previous case. These interchanges yield no new candidates G for stable disarrangement phases, because the formula (33) for G and the formula (78) for H(e, f) are symmetric with respect to interchange of e and f.

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