Stable Disarrangement Phases of Granular Media I: Classification of the Disarrangement Phases of a Model Aggregate

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Abstract

We model granular media as continuous bodies that are aggregates of many small elastic bodies (elastic aggregates). Our model rests on the multiscale geometry of structured deformations through the field theory "elasticity with disarrangements". This setting provides a tensorial consistency relation $D\Psi(G)(F^T - G^T) = 0$ and an accommodation inequality $0 < \det G \leq \det F$ that relate, through the free energy response Ψ of the individual pieces of the aggregate, the deformation gradient F of the aggregate and the average deformation G of the pieces of the aggregate. The solutions G of these two relations are called disarrangement phases corresponding to F. In Part I we classify all of the disarrangement phases for a model elastic aggregate. The compact phase $G = F$, in which the pieces of the aggregate all deform in the same way as the aggregate, itself, forms one category in the classification, while the non-compact phases $G \neq F$ are categorized as to whether the stress $(\det F)^{-1} D\Psi(G)F^T$ is planar, uniaxial, or zero. Our classification will form the basis for the solution of boundary value problems for the model aggregate as well as for a broader class of aggregates. In Part II we use the classification to obtain an unexpected connection between elastic aggregates and materials with no-tension response.

1 Introduction

A principal challenge in modeling 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, 2, 3] the manner in which the macroscopic deformation of an aggregate of elastic bodies, treated as a single, continuous body, can be related to the submacroscopic deformation of the pieces of the aggregate (for other treatments of aggregates see e.g. [4, 5, 6]). Structured deformations provide an appropriate setting, because they provide purely geometrical fields g and 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 [7] of elastic bodies undergoing disarrangements provides the *consistency* relation $\mathcal{C}(F, G) = 0$, a tensorial relation whose form is determined by the Helmholtz free energy response of the body, and 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 this article we define 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.

Our specific goals in Part I of the present study are

- to introduce formally the concept of disarrangement phase in the context of aggregates of elastic bodies,
- to point out in the broadest class of elastic aggregates the existence for each F of a "compact" disarrangement phase, or disarrangement-free phase, in which the pieces of the aggregate deform in the same way as the aggregate, itself,
- to point out in a slightly narrower context the existence for each F with sufficiently large determinant of "loose" disarrangment phases in which each piece of the aggregate relaxes to a stress-free configuration that generally differs from F,
- to determine for a model elastic aggregate a classification of the disarrangment phases, including ones that are neither compact phases nor loose phases.

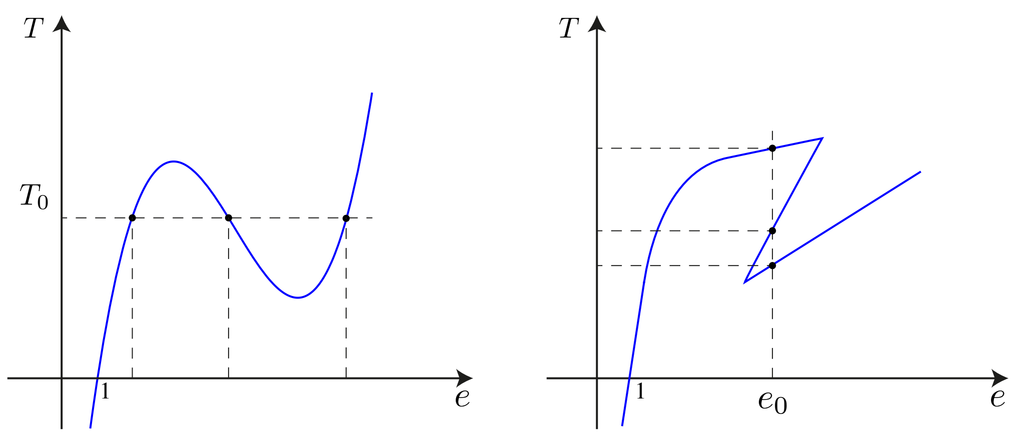

Figure 1: Standard phases and disarrangement phases.

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 the figure "Standard phases and disarrangement phases," 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.

$\square$

In Section 2 we review the aspects of structured deformations and of the field theory "elasticity with disarrangements" [7] 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 consideration do not result in the storage of energy and may be described as "purely dissipative." The consistency relation and the accommodation inequality are recorded there, and, because of the centrality of the consistency relation in this article, we provide in the Appendix to Part II not only a sketch of its derivation but also a simple, submacroscopic interpretation of the consistency relation in the case of purely dissipative disarrangements: *for the case of purely dissipative disarrangements the consistency relation implies that, on average, the tractions vanish at points of the body where submacroscopic slips or separations occur.* We end Section 2 with a proof, based on the consistency relation and a semiconvexity property of Ψ, that, for a given F, disarrangements of rank one cannot increase the free energy density.

Section 3 contains the definition of "disarrangement phase corresponding to F" as well as the description of the compact phase (disarrangement-free phase) and, for a slightly less general class of aggregates, a description of the 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.

We describe in Section 4 a 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, [9], Section 4.10) that determines the model elastic aggregate under study here.

In Section 5 we are able to classify, for a given but arbitrary deformation gradient F, all of the solutions of the consistency relation in terms of the dimensionless ratio $r = \alpha/\beta$. These solutions G naturally form four categories: "compact," "plane-stress," "uniaxial stress." and "stress-free," the last three 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. We also obtain for each category the specific form taken on by the accommodation inequality as well as expressions for the stress, free energy, and the left stretch tensor for G.

The "first-order" structured deformations employed here do not provide an intrinsic length scale that could be used to describe the sizes of the pieces of the aggregate. However, the "second-order" structured deformations introduced in [10] do provide such a length scale and, hence, the possibility of incorporating size effects into models of elastic aggregates. Nevertheless, the present approach based on first-order structured deformations can provide dimensionless geometrical quantities that measure ratios of sizes of pieces of the aggregate to other important characteristic lengths such as the size of shear bands that support large, localized deformations (see e.g. [11, 12, 13, 14]) or the size of compact filaments that substantially bear loads in the aggregate. (See, for example [15], [16], for dimensionless quantities corresponding to first-order structured deformations of single crystals and for the role of these dimensionless quantities in modeling the hardening behavior of aluminium single crystals in Taylor's soft device.)

2 Statics of elastic aggregates

The multiscale geometry provided by structured deformations [1] in the context of a recent field theory of elastic bodies [7] has been applied [17] to describe the dynamics of a continuum composed of small elastic bodies that can deform individually in a manner that differs from the macroscopic deformation of the continuum. Here, we specialize that description to a body that does not evolve in time. In this context, a structured deformation (g, G) provides the *macroscopic deformation* $g : \mathcal{B} \longrightarrow \mathcal{E}$ mapping points X in the body $\mathcal{B}$ injectively into points $g(X)$ in Euclidean space $\mathcal{E}$ as well as the *deformation without disarrangements* $G : \mathcal{B} \longrightarrow Lin$ mapping points X in the body into second-order tensors $G(X)$ that describe the deformation of pieces of the aggregate. 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:

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

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* (see Fig. 2 for illustration). The accomodation inequality can be used to prove the Approximation Theorem [1]: there exists a sequence $n \longmapsto f_n$ of injective, piecewise-smooth mappings of the body into Euclidean space such that

$$g = \lim_{n\longrightarrow\infty} f_n \text{ and } G = \lim_{n\longrightarrow\infty} \nabla f_n \tag{2}$$

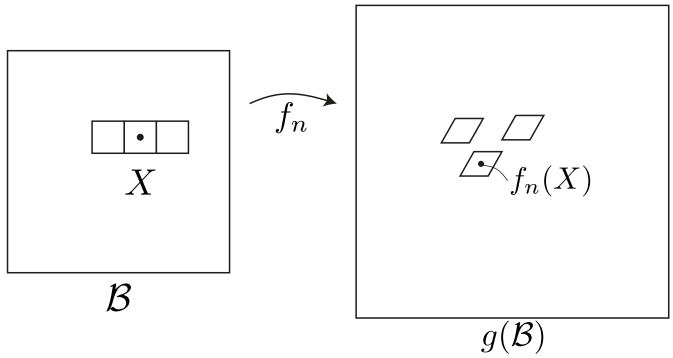

Figure 2: Piecewise smooth deformation f_n and the resulting macroscopic deformation (shearing and separation of individual pieces may result in a macroscopic expansion)

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], [18] 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 *deformation due to disarrangements.* (See the Appendix in Part II for an identification relation that justifies this terminology.) 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 due to disarrangements G and the deformation without disarrangements M [7]. 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 [17] that the Helmholtz free energy field ψ for the aggregate is determined entirely by the deformation without disarrangements G, which at each point X in 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 [2], 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 [7] reduce in statics, and in the present case of purely dissipative disarrangements, to the system

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

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

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

in which (5) is the equation of balance of forces, (6) is a tensorial equation, 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 this article and [7] 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, 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*

$$D\Psi(A) \cdot (a \otimes b) \leq \Psi(A + a \otimes b) - \Psi(A). \tag{9}$$

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 $(g, \nabla g)$:

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

To verify this remark, we note that, from (6), (9), and the fact that $M(X)$ is rank one:

$$\begin{aligned} 0 &= D\Psi(G(X))(\nabla g(X) - G(X))^T \cdot I = D\Psi(G(X)) \cdot (\nabla g(X) - G(X)) \\ &\leq \Psi(G(X) + (\nabla g(X) - G(X))) - \Psi(G(X)) \\ &= \Psi(\nabla g(X)) - \Psi(G(X)). \end{aligned}$$

3 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

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

and on the accommodation inequality (7)

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

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:

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

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. 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 $X \longmapsto X_0 + F(X - X_0)$ and in which each piece undergoes the homogeneous deformation $X \longmapsto X_0 + G(X - X_0)$.

We consider now two widely occurring examples of disarrangement phases. 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 [17]. 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 [17] that, for isotropic free energy response functions Ψ satisfying standard smoothness, semiconvexity and growth properties, there exists a positive number $\varsigma_{\min}$ 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

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

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 $\varsigma_{\min}$ 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.

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

Our aim in the remainder of the paper is to illustrate the richness of possibilities for disarrangement phases of elastic aggregates through the choice of a specific free energy response function that appears widely in the literature (see, for example, [9], Section 4.10) and that also was used for illustrative purposes in our article [17]. We let α and β be positive numbers and consider henceforth an elastic aggregate whose free energy response function is

$$\Psi_{\alpha\beta}(G) = \frac{1}{2}\alpha(\det G)^{-2} + \frac{1}{2}\beta tr(GG^T) = \frac{1}{2}\beta(\frac{r}{\det B_G} + trB_G) \tag{15}$$

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

$$\beta^{-1}S = \beta^{-1}D\Psi_{\alpha\beta}(G) = -\frac{r}{(\det G)^2}G^{-T} + G. \tag{16}$$

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 $b = 0$.

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 I the 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:

$$D\Psi_{\alpha\beta}(G) = 0 \quad \text{if and only if} \quad G = r^{1/8}R \text{ for some rotation } R. \tag{17}$$

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 (15) at such points is given by

$$\frac{2}{\beta}\Psi_{\alpha\beta}(r^{1/8}R) = \frac{r}{r^{3/4}} + tr(r^{1/4}I) = 4r^{1/4}. \tag{18}$$

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

$$r^{3/8} = \det(r^{1/8}R) \leq \det F, \tag{19}$$

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 $X \longmapsto Q(X)$ on the body, the structured deformation $(g, r^{1/8}Q)$ has the property that, at every point X in 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 $G = F$ corresponding to F yields the stress in the reference configuration S satisfying

$$\beta^{-1}S = F - \frac{r}{(\det F)^2}F^{-T} \tag{20}$$

as well as the stress in the deformed configuration T satisfying

$$\begin{aligned} \beta^{-1}(\det F)T &= \beta^{-1}SF^T = FF^T - r(\det(FF^T))^{-1}I \\ &= B_F - r(\det B_F)^{-1}I, \end{aligned} \tag{21}$$

with $B_F = FF^T$.

5 General solutions of the consistency relation associated with $\Psi_{\alpha\beta}$

With a view toward classifying the disarrangement phases of the model material, we focus here first on determining all of the solutions of the consistency relation $(13)_1$, which here, by (20), is equivalent to

$$(G - \frac{r}{(\det G)^2} G^{-T})(F^T - G^T) = 0. \tag{22}$$

Specifically, we let F be given and seek all solutions G with $\det G > 0$ of (22), 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 (22) 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

$$(B_G - \frac{r}{\det B_G} I)(R_G F^T - V_G) = 0. \tag{23}$$

5.1 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 (23) 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 $\Psi_{\alpha\beta}(G)$:

$$\beta^{-1}(\det F)T = FF^T - \frac{r}{(\det F)^2} I \tag{24}$$

$$2\beta^{-1}\Psi_{\alpha\beta}(G) = \frac{r}{(\det F)^2} + tr(FF^T) \tag{25}$$

Of course, in this case the accommodation inequality (7) is satisfied with equality.

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

We assume now that $G \neq F$ and note from (23) 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 non-trivial. 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

$$(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r. \tag{26}$$

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 :

$$B_G = \sum_{i=1}^{3} \lambda_i^G e_i^G \otimes e_i^G \text{ and } V_G = \sum_{i=1}^{3} (\lambda_i^G)^{1/2} e_i^G \otimes e_i^G. \tag{27}$$

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 (23), taking into account (26), and using $I = \sum_{i=1}^{3} e_i^G \otimes e_i^G$ we find that the consistency relation is equivalent to

$$\sum_{i=2}^{3}(\lambda_i^G - \lambda_1^G)e_i^G \otimes e_i^G \left(R_G F^T - \sum_{j=1}^{3}(\lambda_j^G)^{1/2} e_j^G \otimes e_j^G \right) = 0. \tag{28}$$

The identity $(a \otimes b)A = a \otimes A^T b$ and the orthonormality of the basis e_1^G , e_2^G, e_3^G yield the relation

$$\begin{aligned} 0 &= \sum_{i=2}^{3}(\lambda_i^G - \lambda_1^G)e_i^G \otimes (F R_G^T e_i^G - (\lambda_i^G)^{1/2} e_i^G) \\ &= \sum_{i=2}^{3} e_i^G \otimes (\lambda_i^G - \lambda_1^G)(F R_G^T - (\lambda_i^G)^{1/2} I)e_i^G. \end{aligned} \tag{29}$$

Taking the transpose of the last sum of dyads and applying it to each of the basis vectors e_2^G and e_3^G leads to the equivalent system of vector relations

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

while applying it to the basis vector e_1^G yields no new information. In summary, these arguments show: *if* $G \neq F$, *then without loss of generality* $(\lambda_1^G)^2 \lambda_2^G \lambda_3^G = r$, *and the consistency relation is equivalent to (30).*

5.2.1 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

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

Taking the magnitudes of the vectors on both sides of these relations permits us to express two of the eigenvalues of B_G in terms of the action of B_F on eigenvectors of B_G:

$$\begin{aligned} \lambda_i^G &= \left|F^{-1} e_i^G\right|^{-2} = (F^{-1} e_i^G \cdot F^{-1} e_i^G)^{-1} \\ &= (F^{-T} F^{-1} e_i^G \cdot e_i^G)^{-1} = (B_F^{-1} e_i^G \cdot e_i^G)^{-1} \ \text{ for } i = 2, 3, \end{aligned} \tag{32}$$

and, by (26), we also obtain the relation

$$\lambda_1^G = \sqrt{r}(B_F^{-1} e_2^G \cdot e_2^G)^{1/2} (B_F^{-1} e_3^G \cdot e_3^G)^{1/2}. \tag{33}$$

Because (31) gives the action of the rotation R_G^T on the pair of orthogonal unit vectors e_2^G and e_3^G, it follows that

$$\begin{aligned} R_G^T e_1^G &= R_G^T (e_2^G \times e_3^G) = R_G^T e_2^G \times R_G^T e_3^G \\ &= (\lambda_2^G)^{1/2} F^{-1} e_2^G \times (\lambda_3^G)^{1/2} F^{-1} e_3^G \\ &= (\lambda_2^G)^{1/2} (\lambda_3^G)^{1/2} (F^{-1} e_2^G \times F^{-1} e_3^G). \end{aligned}$$

The relation $Av \times Aw = (\det A)A^{-T}(v \times w)$ with $A := F^{-1}$ then implies

$$\begin{aligned} R_G^T e_1^G &= \frac{(\lambda_2^G)^{1/2}(\lambda_3^G)^{1/2}}{\det F} F^T(e_2^G \times e_3^G) \\ &= \frac{(\lambda_2^G)^{1/2}(\lambda_3^G)^{1/2}}{\det F} F^T e_1^G \\ &= \frac{1}{(B_F^{-1}e_2^G \cdot e_2^G)^{1/2}(B_F^{-1}e_3^G \cdot e_3^G)^{1/2} \det F} F^T e_1^G. \end{aligned} \tag{34}$$

For $i = 2, 3$ the original relations (31) can be written by means of (32) in a form similar to (34):

$$R_G^T e_i^G = \frac{1}{(B_F^{-1}e_i^G \cdot e_i^G)^{1/2}} F^{-1} e_i^G. \tag{35}$$

We conclude that the consistency relation (22) in the present case implies the formulas (32) and (33) for the eigenvalues of B_G as well as the formulas (34) and (35) that determine R_G. Moreover, the quantities R_G and $B_G = V_G^2$ determined through these formulas are expressed in terms of the eigenvectors of B_G, together with the actions of B_F^{-1}, of F^{-1}, and of F^T on these eigenvectors. Because R_G is orthogonal, the formula (35) tells us that

$$\begin{aligned} B_F^{-1}e_2^G \cdot e_3^G &= (FF^T)^{-1}e_2^G \cdot e_3^G = F^{-1}e_2^G \cdot F^{-1}e_3^G = \\ &= (V_G R_G)^{-1}e_2^G \cdot (V_G R_G)^{-1}e_3^G \\ &= (\lambda_2^G)^{-1/2}(\lambda_3^G)^{-1/2} R_G^T e_2^G \cdot R_G^T e_3^G = 0 \end{aligned} \tag{36}$$

and, in particular, not only are e_2^G and e_3^G orthogonal, but so also are $F^{-1}e_2^G$ and $F^{-1}e_3^G$.

Writing $G^T = R_G^T V_G$ we may use the results just obtained to write

$$\begin{aligned} G^T &= \sum_{i=1}^{3} (\lambda_i^G)^{1/2} R_G^T e_i^G \otimes e_i^G \\ &= \frac{r^{1/4}}{(B_F^{-1}e_2^G \cdot e_2^G)^{1/4}(B_F^{-1}e_3^G \cdot e_3^G)^{1/4} \det F} F^T e_1^G \otimes e_1^G \\ &\quad + \sum_{i=2}^{3} (B_F^{-1}e_i^G \cdot e_i^G)^{-1} F^{-1} e_i^G \otimes e_i^G, \end{aligned}$$

so that for the present case $\lambda_i^G \neq \lambda_1^G$ for $i = 2, 3$, the consistency relation in its equivalent form (31) yields the following formula

$$\begin{aligned} G &= \frac{r^{1/4}}{(B_F^{-1}e_2^G \cdot e_2^G)^{1/4}(B_F^{-1}e_3^G \cdot e_3^G)^{1/4} \det F} (e_1^G \otimes e_1^G) F \\ &\quad + (\sum_{i=2}^{3} (B_F^{-1}e_i^G \cdot e_i^G)^{-1} e_i^G \otimes e_i^G) F^{-T} \end{aligned} \tag{37}$$

and necessitates that (32) - (36) hold. The condition $\lambda_i^G \neq \lambda_1^G$ for $i = 2, 3$ becomes the restriction

$$\sqrt{r}(B_F^{-1}e_2^G \cdot e_2^G)^{1/2}(B_F^{-1}e_3^G \cdot e_3^G)^{1/2} \neq (B_F^{-1}e_i^G \cdot e_i^G)^{-1} \quad \text{for } i = 2, 3 \tag{38}$$

on two of the eigenvectors e_2^G and e_3^G of B_G. We also note for later use the formula

$$\begin{aligned}\det G &= (\det B_G)^{1/2} = (\frac{r}{\lambda_1^G})^{1/2} \\ &= (\frac{r}{\sqrt{r}(B_F^{-1}e_2^G \cdot e_2^G)^{1/2}(B_F^{-1}e_3^G \cdot e_3^G)^{1/2}})^{1/2} \\ &= \frac{r^{1/4}}{(B_F^{-1}e_2^G \cdot e_2^G)^{1/4}(B_F^{-1}e_3^G \cdot e_3^G)^{1/4}}. \end{aligned} \tag{39}$$

Actually, the relations (32) - (39) just derived yield a characterization of all solutions G 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*

$$F^{-1}e \cdot F^{-1}f = 0, \quad r^{1/2}\left|F^{-1}e\right|^3\left|F^{-1}f\right| \neq 1, \quad r^{1/2}\left|F^{-1}e\right|\left|F^{-1}f\right|^3 \neq 1. \tag{40}$$

Then the tensor

$$\begin{aligned} G &= r^{1/4}\left|F^{-1}e\right|^{1/2}\left|F^{-1}f\right|^{1/2}(e\times f)\otimes(\frac{F^{-1}e}{|F^{-1}e|}\times\frac{F^{-1}f}{|F^{-1}f|})+ \\ &\quad +\left|F^{-1}e\right|^{-1} e\otimes\frac{F^{-1}e}{|F^{-1}e|}+\left|F^{-1}f\right|^{-1} f\otimes\frac{F^{-1}f}{|F^{-1}f|} \end{aligned} \tag{41}$$

is a solution of the consistency relation (31), and the solution (41) equals F if and only if

$$B_F(e\times f) = \frac{r}{\det B_F} e\times f. \tag{42}$$

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 (41) for some choice of the orthogonal unit vectors e and f satisfying (40), and this formula for G implies that

$$\begin{aligned} V_G &= r^{1/4}\left|F^{-1}e\right|^{1/2}\left|F^{-1}f\right|^{1/2}(e\times f)\otimes(e\times f)+ \\ &\quad +\left|F^{-1}e\right|^{-1} e\otimes e+\left|F^{-1}f\right|^{-1} f\otimes f, \end{aligned} \tag{43}$$

$$\begin{aligned} R_G &= (e\times f)\otimes(\frac{F^{-1}e}{|F^{-1}e|}\times\frac{F^{-1}f}{|F^{-1}f|})+ \\ &\quad +e\otimes\frac{F^{-1}e}{|F^{-1}e|}+f\otimes\frac{F^{-1}f}{|F^{-1}f|}, \end{aligned} \tag{44}$$

$$\det G = r^{1/4}\left|F^{-1}e\right|^{-1/2}\left|F^{-1}f\right|^{-1/2}. \tag{45}$$

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

$$\begin{aligned} \beta^{-1}(\det F)T &= \left|F^{-1}e\right|^{-2}(1-\ r^{1/2}\left|F^{-1}e\right|^3\left|F^{-1}f\right|)\, e\otimes e+ \\ &\quad +\left|F^{-1}f\right|^{-2}(1-\ r^{1/2}\left|F^{-1}e\right|\left|F^{-1}f\right|^3)\, f\otimes f, \end{aligned} \tag{46}$$

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

$$\frac{2}{\beta}\Psi_{\alpha\beta}(G) = 2r^{1/2}\left|F^{-1}e\right|\left|F^{-1}f\right| + \left|F^{-1}e\right|^{-2} + \left|F^{-1}f\right|^{-2}. \tag{47}$$

We note that the formula (43) for V_G immediately yields the formulas

$$\begin{aligned}
\lambda_1^G &= (r^{1/4}\left|F^{-1}e\right|^{1/2}\left|F^{-1}f\right|^{1/2})^2 = r^{1/2}\left|F^{-1}e\right|\left|F^{-1}f\right|, \\
\lambda_2^G &= (\left|F^{-1}e\right|^{-1})^2 = \left|F^{-1}e\right|^{-2}, \\
\lambda_3^G &= (\left|F^{-1}f\right|^{-1})^2 = \left|F^{-1}f\right|^{-2}
\end{aligned} \tag{48}$$

for the eigenvalues of the stretch tensor $B_G = V_G^2$, and it follows directly that these eigenvalues satisfy the relation (26). Moreover, the corresponding eigenvectors e_1^G, e_2^G, e_3^G of B_G (and of V_G) are $e \times f$, e, and f, respectively. It is clear that the right-hand sides of the formulas (43) and (44) are, respectively, positive definite and orthogonal tensors and that their product is the right-hand side of (41). This observation allows us to verify the consistency relation using the equivalent form (31) along with (43), (44), and (48):

$$R_G^T e_2^G = R_G^T e = \frac{F^{-1}e}{|F^{-1}e|} = (\lambda_2^G)^{1/2}F^{-1}e$$

with a similar calculation showing that $R_G^T e_3^G = (\lambda_3^G)^{1/2}F^{-1}f$. With these observations, we have verified that the formula (41) does in fact provide a solution to the consistency relation, and the arguments that yielded above the relations (32) - (39) show that every solution G in this case has the form (41). It is clear from (26) that (42) is a necessary condition for the equality of G in (41) and F. The sufficiency of (42) for this equality is established by showing that (42), (41), and $(40)_1$ imply that $F^{-1}G = I$, and we omit the details of this argument. To complete the verification of the remark, we note that

$$\begin{aligned}
\beta^{-1}(\det F)T &= D\Psi_{\alpha\beta}(G)F^T = D\Psi_{\alpha\beta}(G)G^T \\
&= (G - \tfrac{r}{(\det G)^2}G^{-T})G^T = V_G^2 - \tfrac{r}{(\det G)^2}I \\
&= (r^{1/4}\left|F^{-1}e\right|^{1/2}\left|F^{-1}f\right|^{1/2})^2(e\times f)\otimes(e\times f) + \\
&\quad \left|F^{-1}e\right|^{-2} e\otimes e + \left|F^{-1}f\right|^{-2} f\otimes f - r^{1/2}\left|F^{-1}e\right|\left|F^{-1}f\right| I
\end{aligned}$$

which when simplified gives the formula (46), and we note, finally, that (47) follows from the definition (15) of $\Psi_{\alpha\beta}$ and from (48). (The second equation used in the calculation above is nothing other than the consistency relation, itself).

The formula (46) 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 (41) of the consistency relation in the present case $\lambda_i^G \neq \lambda_1^G$ for $i = 2, 3$, and we shall 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 $0 < \det G \leq \det F$:

$$0 < r^{1/4}\left|F^{-1}e\right|^{-1/2}\left|F^{-1}f\right|^{-1/2} \leq \det F. \tag{49}$$

5.2.2 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

$$R_G^T e_3^G = (\lambda_3^G)^{1/2} F^{-1} e_3^G \tag{50}$$

and using the same reasoning as in (32) we have

$$\lambda_3^G = (B_F^{-1} e_3^G \cdot e_3^G)^{-1} = \left|F^{-1} e_3^G\right|^{-2}, \tag{51}$$

and, by (26) and $\lambda_2^G = \lambda_1^G$ we immediately obtain the formulas

$$(\lambda_1^G)^3 = \frac{r}{\lambda_3^G} = r(B_F^{-1} e_3^G \cdot e_3^G) = r\left|F^{-1} e_3^G\right|^2,$$

$$\lambda_1^G = \lambda_2^G = r^{1/3}(B_F^{-1} e_3^G \cdot e_3^G)^{1/3} = r^{1/3}\left|F^{-1} e_3^G\right|^{2/3}, \tag{52}$$

$$\begin{aligned} \det B_G &= \frac{r}{\lambda_1^G} = \frac{r^{2/3}}{(B_F^{-1} e_3^G \cdot e_3^G)^{1/3}} = \left(\frac{r}{\left|F^{-1} e_3^G\right|}\right)^{2/3}, \\ \det G &= (\det B_G)^{1/2} = \frac{r^{1/3}}{(B_F^{-1} e_3^G \cdot e_3^G)^{1/6}} = \left(\frac{r}{\left|F^{-1} e_3^G\right|}\right)^{1/3}. \end{aligned} \tag{53}$$

We note here that the condition $\lambda_3^G \neq \lambda_1^G$ in the definition of the present case now takes the form $\left|F^{-1} e_3^G\right|^{-2} \neq r^{1/3}\left|F^{-1} e_3^G\right|^{2/3}$, i.e.,

$$r\left|F^{-1} e_3^G\right|^8 \neq 1. \tag{54}$$

The relation (50) now becomes

$$R_G^T e_3^G = \left|F^{-1} e_3^G\right|^{-1} F^{-1} e_3^G \tag{55}$$

and we may write along the lines of the argument in the previous subsection:

$$\begin{aligned} G^T &= \sum_{i=1}^{3} (\lambda_i^G)^{1/2} R_G^T e_i^G \otimes e_i^G \\ &= \sum_{i=1}^{2} (\lambda_i^G)^{1/2} R_G^T e_i^G \otimes e_i^G + (\lambda_3^G)^{1/2} R_G^T e_3^G \otimes e_3^G \\ &= r^{1/6}\left|F^{-1} e_3^G\right|^{1/3} R_G^T \sum_{i=1}^{2} e_i^G \otimes e_i^G + \left|F^{-1} e_3^G\right|^{-1}\left|F^{-1} e_3^G\right|^{-1} F^{-1} e_3^G \otimes e_3^G. \end{aligned}$$

Taking the transpose of both sides of this relation leads us to the following formula for G:

$$G = r^{1/6}\left|F^{-1} e_3^G\right|^{1/3}\left(\sum_{i=1}^{2} e_i^G \otimes e_i^G\right) R_G + \left|F^{-1} e_3^G\right|^{-2} (e_3^G \otimes e_3^G) F^{-T},$$

or, alternatively, writing $\sum_{i=1}^{2} e_i^G \otimes e_i^G = I - e_3^G \otimes e_3^G$, we are led to the relation

$$G = r^{1/6}\left|F^{-1} e_3^G\right|^{1/3}\left(I - e_3^G \otimes e_3^G\right) R_G + \left|F^{-1} e_3^G\right|^{-1} e_3^G \otimes \frac{F^{-1} e_3^G}{\left|F^{-1} e_3^G\right|}. \tag{56}$$

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

$$R^T e = \frac{F^{-1}e}{|F^{-1}e|} \qquad \text{and} \qquad r^{1/8}\left|F^{-1}e\right| \neq 1. \tag{57}$$

Then the tensor G given by

$$G = r^{1/6}\left|F^{-1}e\right|^{1/3}(I - e\otimes e)\,R + \left|F^{-1}e\right|^{-1} e \otimes \frac{F^{-1}e}{|F^{-1}e|} \tag{58}$$

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 (56) equals F if and only if $R_F = R$ and, for all vectors v perpendicular to e,

$$B_F\, v = \frac{r}{\det B_F} v. \tag{59}$$

Moreover, every solution of the consistency relation for this case is of the form (58) with R and e satisfying (57), and the following relations hold:

$$\begin{aligned} V_G &= r^{1/6}\left|F^{-1}e\right|^{1/3}(I - e\otimes e) + \left|F^{-1}e\right|^{-1} e\otimes e && (60)\\ R_G &= R && (61)\\ \det G &= \det V_G = r^{1/3}\left|F^{-1}e\right|^{-1/3} && (62)\end{aligned}$$

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

$$\beta^{-1}(\det F)T = \frac{1 - r^{1/3}\left|F^{-1}e\right|^{8/3}}{\left|F^{-1}e\right|^2} e\otimes e, \tag{63}$$

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

$$\frac{2}{\beta}\Psi_{\alpha\beta}(G) = 3r^{1/3}\left|F^{-1}e\right|^{2/3} + \left|F^{-1}e\right|^{-2}. \tag{64}$$

To verify (60) and (61), it suffices to use (57) to rewrite (58) in the form

$$\begin{aligned} G &= r^{1/6}\left|F^{-1}e\right|^{1/3}(I - e\otimes e)\,R + \left|F^{-1}e\right|^{-1} e\otimes \frac{F^{-1}e}{|F^{-1}e|}\\ &= r^{1/6}\left|F^{-1}e\right|^{1/3}(I - e\otimes e)\,R + \left|F^{-1}e\right|^{-1} e\otimes R^T e\\ &= (r^{1/6}\left|F^{-1}e\right|^{1/3}(I - e\otimes e) + \left|F^{-1}e\right|^{-1} e\otimes e)R \end{aligned}$$

and to note that the second factor on the right is the rotation R and the first factor is positive definite and symmetric. The satisfaction of the consistency relation in the form (50) by the tensor G in (58) then follows from (57) and the fact that $V_G e = \left|F^{-1}e\right|^{-1} e$. The assertion containing the relation (59) is easily verified by employing the polar decomposition of G below (64) and the uniqueness of the factors in that decomposition. That every solution of the consistency relation in the present case is of the form (58) is established by the arguments that precede the statement of the Remark, and the formulas (63) and (64) are then easily verified.

The formula (63) and the restriction (57) 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 (7) in the form $0 < \det G \leq \det F$:

$$0 < r^{1/3} \left|F^{-1}e\right|^{-1/3} \leq \det F. \tag{65}$$

5.2.3 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 (26) immediately yields $\lambda_1^G = \lambda_2^G = \lambda_3^G = r^{1/4}$, so that

$$B_G = r^{1/4} I \quad \text{and} \quad G = r^{1/8} R, \tag{66}$$

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

$$\det G = r^{3/8}, \tag{67}$$

and we note that this case recovers precisely those tensors G identified in 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

$$T = 0 \quad \text{and} \quad 2\beta^{-1}\Psi_{\alpha\beta}(G) = 4r^{1/4}, \tag{68}$$

and the accommodation inequality (7) takes the form

$$r^{3/8} \leq \det F. \tag{69}$$

6 Conclusions

In this Part I of our study we have delimited the coupling between the macroscopic deformation F and the deformation G of the pieces (or grains) of an elastic aggregate through the consistency relation $D\Psi(G)(F^T - G^T) = 0$ and through the accommodation inequality $0 < \det G \leq \det F$. For a model elastic aggregate and for a given but arbitrary F, we have classified all of the solutions G of these two relations (the disarrangement phases corresponding to F) according to whether $G = F$ (the compact phase in which all of the pieces of the aggregate deform in the same way as the aggregate) or $G \neq F$. Three categories exhaust the class of non-compact phases $G \neq F$, corresponding to whether the Cauchy stress $T = (\det F)^{-1} D\Psi(G)F^T$ is planar, uniaxial, or zero. The four categories of disarrangement phases provide a rich portfolio of phases that can appear in response to prescribed boundary conditions on the aggregate, and future research will employ these phases in the solution of a variety of boundary-value problems. The classification also provides a basis for the study of stable disarrangement phases of the model aggregate that we provide in Part II. That study achieves an unexpected connection between elastic aggregates and the no-tension materials used to describe structures composed of masonry-like elements.

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