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# Disarrangements in Continua and the Geometry of Microstructure

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## Dedicated to Professor T. C. Woo on the occasion of his retirement

**Abstract**

The term "disarrangement" is proposed here to describe geometrical changes either at the macroscale or at the microscale that are not accounted for by the classical deformations employed in continuum mechanics. Collections of non-classical deformations studied by Del Piero and Owen (1993) are then described in order to give a more precise context for the term "disarrangement". Examples of disarrangements both at the microscale and at the macroscale are presented, including disarrangements in liquid crystals, metallic crystals, and mixtures of continua. It is shown that volume-preserving deformations that are limits of discrete translations in crystallographically preferred directions necessarily are "piecewise-shearing deformations".

# 1. Introduction

The purpose of this paper is to propose some alternative terminology and to provide expanded interpretation for geometrical concepts and results obtained in a recent study of continuum deformations that describe changes in microstructure (Del Piero and Owen (1993)). In that study, the authors introduced and analyzed collections of non-classical deformations, and then applied their results to describe the geometry of elastic and plastic deformations in metals, the changes of molecular orientation fields in liquid crystals, the changes of lattice bases fields describing the lattice structure of crystals with defects, and some aspects of mixing continua. These geometrical changes were described using such terms as "macrofracture", "microfracture", and "fracture zone" that conveyed accurately the geometrical nature of many macro- and microstructural changes. However, the term "fracture" is widely used by engineers working in the field of fracture mechanics to describe permanent, usually irreversible geometrical changes; therefore, the term "fracture" carries a special connotation that is not appropriate to many of the applications envisaged in Del Piero and Owen (1993). For example, the movement of an edge dislocation through through a crystal causes a relocation of part of the atomic lattice, without introducing a weakening or damage as would be suggested by use of the term "fracture". Similarly, plastic deformation in a metal involves geometrical changes that are supported on many, widely dispersed, thin zones in the metal and that need not entail damage or mechanical fracture, even at the microscopic level.

The fact that the term "fracture" has a specific and already accepted connotation in mechanics led O. Richmond and K. Rajagopal (independently) to suggest that a different, more neutral term be chosen to describe the wide range of geometrical changes embodied in the deformations studied by Del Piero and Owen (1993). Ideally, in this broader context, any candidate for such a term should cover not only non-smooth changes at the macroscopic level, such as separation of a body into pieces, but also diverse aspects of microstructural changes, including dislocation, discrete and continuous slip, creation of voids, dispersion, diffusion, evaporation, and condensation. Here, I propose the term "disarrangement" (literally, the upsetting of an arrangement) to describe such geometrical changes that can accompany continuum deformations. Specifically, I propose that the term "fracture" as used by Del Piero and Owen be replaced by the term disarrangement, and that the terms "fractured zone", "macrofracture", and "microfracture" be replaced, respectively, by the terms "disarrangement zone", "macrodisarrangement", and "microdisarrangement". (Alternatives for other terms related to "fracture" used by Del Piero and Owen (1993) will be given in subsequent sections of this paper.)

With these proposed alternatives set forth, it remains here to give specific mathematical descriptions of disarrangements, to interpret some of the mathematical results available for them in the context of general continua, and to indicate a variety of application to specific continua. The mathematical content of this paper will be described with a *minimum* of formal definitions, theorems, and proofs, because an extensive mathematical treatment is available in Del Piero and Owen

(1993). It is hoped that the present, more informal treatment will permit emphasis to be laid on the broad scope of these mathematical concepts as tools for describing disarrangements in continua. The applications treated in Sections 3, 4.1, and 5 are translations of the treatments by Del Piero and Owen into the alternative terminology of disarrangements, while the application to structured slip discussed in Section 4.2 is new. In particular, I show in Section 4.2 that volume-preserving deformations that are limits of discrete translations in crystallographically preferred directions necessarily are "piecewise-shearing deformations".

## 2. Non-classical deformations that support disarrangements

The description of "structured deformations", the main class of deformations covered in the present approach to the geometry of microstructure, requires first a description of "classical deformations" and "piecewise-classical deformations". A *classical deformation* from a region $\mathcal{A}$ in physical space $\mathcal{E}$ is an injective, orientation preserving mapping $f$ from $\mathcal{A}$ into $\mathcal{E}$ such that $f$ has an extension to all of $\mathcal{E}$ that is smooth and has a smooth inverse. For each point $x$ in $\mathcal{A}$, $f(x)$ is the location of $x$ in the classical deformation $f$. A classical deformation $f$ is intended to describe smooth, macroscopic, geometrical changes in a continuous body; its gradient $\nabla f$ is a tensor field whose value $\nabla f(x)$ at a point $x$ in $\mathcal{A}$ describes the local, macroscopic, geometrical changes near $x$.

A *piecewise-classical deformation*, or, more briefly, a *simple deformation* from a region $\mathcal{A}$ is specified by giving a subset $\kappa$ of $\mathcal{A}$, called the *activation site* (instead of "crack site", used by Del Piero and Owen (1993)) and a mapping $f$ from $\mathcal{A}\backslash\kappa$

into $\mathcal{E}$, called the *transplacement.* The set $\kappa$ is required to have volume zero, $f$ is required to be injective, and the region $\mathcal{A}\backslash\kappa$ is required to be a finite (not necessarily disjoint) union of regions $\mathcal{A}_j$, $j = 1, ..., J$, such that the restriction $f_j$ of $f$ to each region $\mathcal{A}_j$ is a classical deformation. We may view $\kappa$ as a collection of cuts in the body $\mathcal{A}$ and each restriction $f_j$ as a smooth deformation of a piece of the body. Thus, a simple deformation $(\kappa, f)$ can separate a body, partially or entirely, into pieces and can deform each piece separately; the pieces can come into contact after deformation, but, because $f$ is injective, cannot interpenetrate. Moreover, the restrictions $f_j$ and their gradients $\nabla f_j$ need not extend continuously from one piece $\mathcal{A}_j$ to another. Each simple deformation is intended to describe macroscopic, geometrical changes in a body that arise when all or a portion of the body is disconnected through slip or separation. Such drastic geometrical changes occur at the activation site and will be referred to as *disarrangements at the macroscopic level* or, more briefly, as *macrodisarrangements.*

A *structured deformation* from $\mathcal{A}$ is defined to be a triple $(\kappa, g, G)$ in which $(\kappa, g)$ is a simple deformation from $\mathcal{A}$, and $G$ is a tensor field on $\mathcal{A}\backslash\kappa$ having the same smoothness as $\nabla g$ and satisfying the conditions: there exists a positive number $m$ such that

$$m < \det G(x) \leq \det \nabla g(x) \tag{2.1}$$

at each $x$ in $\mathcal{A}\backslash\kappa$. Before giving interpretations and terminology for the ingredients in structured deformations, we mention some mathematical results for structured and simple deformations obtained by Del Piero and Owen (1993). The collection

of all simple deformations Sid and the collection of all structured deformations Std each has a rather natural notion of composition, each collection has a neutral element, i.e., an element that produces no effect when composed with another deformation, and each collection has a readily identifiable collection of invertible elements (denoted by Inv Sid and Inv Std, respectively). The invertible simple deformations turn out to be those for which the activation site $\kappa$ is the empty set $\emptyset$, and the invertible structured deformations turn out to be those for which not only is the activation site empty, $\kappa = \emptyset$, but also $\det G = \det \nabla g$.

The most striking mathematical result concerning Sid and Std, the Approximation Theorem, Del Piero and Owen (1993), asserts that every structured deformation $(\kappa, g, G)$ is a "limit of simple deformations" in the following sense: for each $(\kappa, g, G)$in Std, there exists a sequence $m \longmapsto (\kappa_m, f_m)$ of simple deformations such that

$$\lim_{m\to\infty} f_m = g, \ \lim_{m\to\infty} \nabla f_m = G, \ \text{ and } \ \lim_{m\to\infty} \inf \kappa_m = \kappa. \tag{2.2}$$

(Here, convergence of $f_m$ and $\nabla f_m$ is in the sense of $L^\infty(\mathcal{A})$, and $\lim_{m\to\infty} \inf \kappa_m := \bigcup_{m=1}^{\infty} \bigcap_{j=m}^{\infty} \kappa_j$.) Thus, in a structured deformation, the mapping $g$ can be obtained as a limit of the transplacements of simple deformations, and the tensor field $G$ can be obtained as a limit of the gradients of those transplacements. Moreover, because the activation sites can split the region $\mathcal{A}$ into pieces, it is not generally true that $\nabla g$ and $G$ are equal. The discrepancy between $G$ and $\nabla g$ reveals a difference between the local deformation due to smooth changes away from activation sites, measured by $G$, and the local deformation at the macroscopic level, measured by

$\nabla g$. Therefore, I will call $G$ the *deformation without disarrangements*; moreover, results proved in Del Piero and Owen (1993) and Del Piero and Owen (1994) show that $\nabla g - G$ is a density for transplacements due to microdisarrangements, i.e., disarrangements at the microlevel. (In these articles, the term "microfracture" was employed in place of microdisarrangement.) These results also show that, for a simple deformation $(\kappa, f)$ and for a structured deformation $(\kappa, g, G)$, transplacements due to macrodisarrangements are given in terms of the jumps in the transplacements $f$ and $g$, respectively. Thus, the concepts and results in Del Piero and Owen (1993) show that the collection Std of structured deformations is rich enough to describe disarrangements at both the macroscopic and microscopic levels and to provide specific measures of deformation with and without disarrangements at both levels. (For a discussion of concepts of stress with and without disarrangements, see the article by Owen (1992) in which the special case of disarrangements due to slip is studied.)

## 3. Disarrangements in liquid crystals

The anisotropic optical and electrical properties of certain liquids can be ascribed to geometrical aspects of the microstructure of these substances: the molecules are nearly rigid, rod-like structures whose axes tend to align in groups. The changes in this geometry as the liquid deforms or is placed in an electric field are instances of microdisarrangements. A simple method of describing these disarrangements in terms of structured deformations rests on the following idea: the collection of all the molecules in a sample of the liquid crystal is depicted first

in a special reference configuration $\mathcal{A}$ with the property that all the molecules have the same alignment, described mathematically as a single unit vector $k$. A sequence of macrodisarrangements of this continuum is effected by choosing a sequence of simple deformations in which the $m^{\text{th}}$ term $(\kappa_m, f_m)$ is a piecewise-rigid deformation that imparts a rigid deformation to each molecule (which generally varies from molecule to molecule). The finitely many values of the unit vector field $(\nabla f_m)\, k$ describe the orientations of the different molecules as a result of the simple deformation $(\kappa_m, f_m)$. One assumes now that the sequence of simple deformations converges in the sense of relation (2.2) to a structured deformation $(\kappa, g, G)$. Because $\nabla f_m$ is orthogonal-valued for each $m$, the limit $G$ of these gradients is orthogonal-valued, so that the vector-field $Gk$ is a unit vector field defined on the region $\mathcal{A}\backslash\kappa$. The unit vector $G(x)\, k$ can be shown to be the limiting value as $m$ tends to infinity of the average of orientations $(\nabla f_m(y))\, k$ of the molecules within a sphere of radius $1/m$ centered at $x$ (Del Piero and Owen (1993)). The vector field $Gk$ is called the *director field* for the liquid crystal (in the configuration determined by $(\kappa, g, G)$). The macroscopic configuration of the liquid crystal is determined by the transplacement $g$, and the local macroscopic deformation is given by the tensor field $\nabla g$, which need not coincide with $G$. Thus, a principal feature of microdisarrangements in a liquid crystal, the director field, is captured precisely by a structured deformation $(\kappa, g, G)$ in which the deformation without disarrangements $G$ is orthogonal-valued. The changes in microstructure are conveyed by the differences between the unit vector $k$ giving the common alignment of molecules in the reference configuration and the unit vectors $G(x)k$ giving the

average alignment of molecules in the deformed configuration. The disarrangement zone is the portion of the reference configuration where $G$ and $\nabla g$ differ: in this zone, the changes in alignment of molecules caused by the deformation are not accounted for by the macroscopic deformation $g$ and the local macroscopic deformation $\nabla g$.

# 4. Disarrangements in metals

## 4.1. Defects in crystals

The ability of a metallic single crystal to undergo large deformations at levels of applied stress well below those predicted from the elastic properties of the material can be ascribed to geometrical aspects of the microstructure of the crystals: the lattice structure formed by the atoms of the metal is not perfect, and the presence and evolution of defects in this structure provides the mechanism for unexpectedly large continuum deformations. Changes in the position and nature of such defects are instances of microdisarrangements. Such disarrangements can most easily be described in terms of structured deformations by depicting the metal in a special reference configuration $\mathcal{A}$ with the property that there are three (not necessarily orthogonal or unit), linearly independent vectors $a, b$, and $c$ such that all of the line segments joining each atom to its nearest neighbors are parallel to one of these three vectors. A sequence of macrodisarrangements of the body is effected by choosing a sequence of simple deformations in which the $m^{\text{th}}$ term $(\kappa_m, f_m)$ is a piecewise-affine deformation that imparts an affine deformation to each of the

basic cells of the atomic lattice; the affine deformation may, of course, vary from one cell to another. For each positive integer $m$, the triple of linearly independent vectors $(\nabla f_m(x))\,a$, $(\nabla f_m(x))\,b$, $(\nabla f_m(x))\,c$ then will take on only finitely many values as $x$ varies over $\mathcal{A}\backslash\kappa_m$. These values describe the change in geometry of the basic cells and, hence, the changes in the lattice structure associated with the simple deformation $(\kappa_m, f_m)$. One assumes now that the sequence of simple deformations converges in the sense of relation (2.2) to a structured deformation $(\kappa, g, G)$. The relation (2.1) guarantees that, for each $x$ in $\mathcal{A}\backslash\kappa$, the triple of vectors $G(x)a$, $G(x)b$, $G(x)c$ is linearly independent. Each of these vectors can be shown to be the limiting value as $m$ tends to infinity of the average of the corresponding vectors $(\nabla f_m(y))\,a$, $(\nabla f_m(y))\,b$, $(\nabla f_m(y))\,c$ as $y$ varies within a sphere of radius $1/m$ centered at $x$ (Del Piero and Owen (1993)). The corresponding vector fields $Ga$, $Gb$, $Gc$ are called the lattice vector fields for the crystal in the configuration determined by $(\kappa, g, G)$. The macroscopic configuration of the crystal is determined by $g$, and the local macroscopic configuration of the crystal is determined by $\nabla g$, which differs generally from $G$. In other words, the images $(\nabla g)\,a$, $(\nabla g)\,b$, $(\nabla g)\,c$ of the lattice directions $a$, $b$, $c$ in the reference configuration need not be the same as the lattice vector fields $Ga$, $Gb$, $Gc$. The closure of the region within $\mathcal{A}\backslash\kappa$ in which at least one of $(\nabla g)\,a$, $(\nabla g)\,b$, $(\nabla g)\,c$ differs from the corresponding field $Ga$, $Gb$, $Gc$, is the disarrangement zone for the structured deformation $(\kappa, g, G)$. Within this zone, the macroscopic deformation $g$ and its gradient $\nabla g$ do not suffice to describe all the change in microstructure occurring in the crystal.

The vector fields $Ga$, $Gb$, and $Gc$ correspond to the lattice vector fields used by Davini and Parry (1989) and Fonseca and Parry (1992) to study the geometry of defects in crystals. Further connections between these, other articles and the present approach are made in Section 7c of Del Piero and Owen (1993).

### 4.2. Structured slip

The framework afforded by structured deformations in Section 4.1 will now be specialized to the case where the simple deformations $(\kappa_m, f_m)$, $m = 1, 2, ...$ that determine a structured deformation $(\kappa, g, G)$ of the crystal all are locally translations in preferred directions determined by the specific atomic structure of the crystal. For example, in f.c.c. crystals, these preferred directions form a set of twelve directions, usually grouped according to which of four possible octahedral planes is parallel to a given translation. Thus, we assume there are given a finite set $S = (u_1, u_2, ..., u_K)$ of unit vectors and a sequence of simple deformations $(\kappa_m, f_m)$, $m = 1, 2, ...$ such that each of the transplacements $f_m$, when restricted to a suitable subregion $\mathcal{A}_{m,j}$ of $\mathcal{A}$, is a translation $f_{m,j}$ of the form

$$f_{m,j}(x) = x + \alpha_{m,j} n_{m,j} \tag{4.1}$$

for $j = 1, 2, ..., J_m$ and $x$ in $\mathcal{A}_{m,j}$. Here, $\alpha_{m,j}$ is a real number that determines the magnitude of the translation, and each unit vector $n_{m,j}$ is in the given set $S$. We assume, in addition, that the transplacement $g$ for the structured deformation $(\kappa, g, G)$ is volume-preserving, so that

$$\det \nabla g = 1. \tag{4.2}$$

We shall now discuss, without supplying many of the mathematical details, the consequences for $(\kappa, g, G)$ of (2.2) (which restricts all structured deformations), (4.1) and (4.2). These results will justify use of the term "structured slip" for a structured deformation $(\kappa, g, G)$ that satisfies (4.1) and (4.2). Let $x$ in $\mathcal{A}\backslash\kappa$ be given such that $g(x) \neq x$. It follows from (4.1) and the first relation in (2.2) that there is a unit vector $u(x)$ in $S$ and a non-zero real number $\alpha(x)$ such that

$$g(x) = x + \alpha(x)u(x). \tag{4.3}$$

Moreover, because $g$ is continuously differentiable on $\mathcal{A}\backslash\kappa$ and the set of points $x$ in $\mathcal{A}\backslash\kappa$ for which $g(x) \neq x$ is open, we conclude that the mappings $x \longmapsto \alpha(x)$ and $x \longmapsto u(x)$ are continuously differentiable. Moreover, because $u(x)$ lies in the finite set $S$, the mapping $x \longmapsto u(x)$ is locally constant. Therefore, we may differentiate relation (4.3) to obtain the formula

$$\nabla g(x) = I + u(x) \otimes \nabla \alpha\,(x) \tag{4.4}$$

in which, as above, $x \longmapsto u(x)$ is locally constant and I denotes the identity tensor. Relations (4.2) and (4.4) now tell us that the vectors $u(x)$ and $\nabla\alpha(x)$ are othogonal. Consequently, on the set of points $x$ for which $g\,(x) \neq x$, the transplacement $g$ is locally a shearing deformation. Each plane on which $\alpha(x)$ is constant undergoes a rigid translation of amount $\alpha(x)$ in the direction $u(x)$. Finally, the second relation in (2.2) and relation (4.1) yield the simple relation $G(x) = I$, for all $x$ in $\mathcal{A}\backslash\kappa$.

In summary, a structured slip turns out to be a structured deformation of the form $(\kappa, g, I)$ in which the transplacement $g$ is a "piecewise-shearing defor-

mation", where the displacements of each of the individual shears are parallel to one of the unit vectors in $S$. In addition, there can be one region in the body on which $g$ is the identity mapping, i.e., on which the displacement of points is zero. The investigation of the geometry of the individual regions on which a shearing deformation occurs or on which no displacement occurs awaits further study. At the moment, it seems reasonable to conjecture that these regions are bounded by the slip planes associated with the given crystal and by the boundary of the body.

## 5. Disarrangements in mixing continua

The act of mixing two or more constituents often involves an intermingling of the constituents at microscopic length scales. In order for the intermingling to occur, at least one constituent must undergo perceptible changes such as dispersion in space, and it is reasonable to conceive of such changes as disarrangements at the microlevel. At macroscopic length scales, mixing generally entails the interpenetration of the constituents. The framework of simple deformations and limits of simple deformations introduced in Section 2 permits us to capture both the intermingling without interpenetration at the microscale and the interpenetration at the macroscale that appear necessary to obtain a comprehensive geometrical description of mixing. The distinction betwen intermingling and interpenetration to be employed below rests on the mathematical distinction between an injective mapping and a non-injective mapping.

We consider each of the $N$ constituents of a mixture as occupying its own reference configuration $\mathcal{A}_j$, $j = 1, 2, ..., N$. The process of intermingling the con-

stituents without interpenetration is described by giving a sequence of simple deformations $(\kappa_m, f_m)$, $m = 1, 2, \ldots$. Each transplacement $f_m$ is an injective mapping whose domain is the region $\mathcal{A}\backslash\kappa_m$, where here $\mathcal{A}$ denotes the union of the regions $\mathcal{A}_j$. The sequence of simple deformations will be said to determine a *mixing deformation* from $\mathcal{A}$ if (i) the sequence of activation sites $\kappa_m$, of transplacements $f_m$ and of their gradients $\nabla f_m$ converge in the sense of (2.2) to $\kappa, g$, and $G$, with the mappings $g$ and $G$ both defined on $\mathcal{A}\backslash\kappa$, and (ii) the restrictions $g_j$ and $G_j$ of $g$ and $G$ to each constituent region $\mathcal{A}_j\backslash\kappa$, are such that the triple $(\kappa \cap \mathcal{A}_j,\ g_j,\ G_j)$ is a structured deformation from $\mathcal{A}_j$. Thus, each consituent undergoes a structured deformation $(\kappa \cap \mathcal{A}_j,\ g_j,\ G_j)$ that permits microdisarrangements such as dispersion in space to occur, each simple deformation $(\kappa_m, f_m)$ intermingles the constituents without interpenetration, and the limit of simple deformations $(\kappa, g, G)$, in which the transpacement $g$ need not be injective, permits the constituents to interpenetrate. The disarrangement zone for the structured deformation $(\kappa \cap \mathcal{A}_j,\ g_j,\ G_j)$ may be described here as the zone of dispersion for the $j^{\text{th}}$ constituent. For each point $y$ in the region $g_j(\mathcal{A}_j\backslash\kappa)$ occupied in space by the $j^{\text{th}}$ constituent of the mixture, the point $x = g_j^{-1}(y)$ represents the material point of the $j^{\text{th}}$ constituent that is present at $y$. In this case, the ratio $\det G_j(x) \,/\, \det \nabla g_j(x)$ is the volume fraction at $y$ of the $j^{\text{th}}$ constituent in the mixing deformation $(\kappa, g, G)$. If a point $y$ in space is not in the region $g_j(\mathcal{A}_j\backslash\kappa)$, the volume fraction at $y$ of the $j^{\text{th}}$ constituent is taken to be zero. (This definition of volume fraction takes into account in the denominator any voids that are present in the mixture as a whole.)

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