

Invertible Structured Deformations and the Geometry of Multiple Slip in Single Crystals

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March 10, 2000

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1 Introduction

Our goal in this paper is to provide counterparts of the basic kinematical relations for incremental slip in single crystals (Bassani, 1993, eqns (2.3) and (2.8)) through derivations that are independent of any notion of intermediate

configuration and are purely geometrical. The geometrical setting of structured deformations (Del Piero & Owen, 1993) employed here permits us to identify rigorously at the outset the part G of the macroscopic deformation F that is due to smooth deformations at smaller length scales. One then deduces that $M = F - G$ is the part of the macroscopic deformation that is due to “disarrangements”, i.e., due to non-smooth deformations at smaller length scales. The further condition $\det F = \det G$ that defines an *invertible* structured deformation (Del Piero & Owen, 1993) permits us to specify that there be no volume change due to disarrangements. Our method for deriving the basic kinematical relations for slip consists of (i) the identification in the usual manner of a finite set of crystallographic diads $s^{(a)} \otimes m^{(a)}$ associated with the geometry of the crystal in a given reference configuration, (ii) the approximation of the disarrangement tensor M by a tensor in the subspace $\mathcal{C}(G)$ spanned by the diads $Gs^{(a)} \otimes m^{(a)}$, (iii) the approximation of the disarrangement tensor $M_t(\tau)$ at time τ , relative to the configuration at time t , by a tensor in the subspace $\mathcal{C}(G_t(\tau))$ spanned by the diads $G_t(\tau)s^{(a)}(t) \otimes m^{(a)}(t)$, with $s^{(a)}(t) = G(t)s^{(a)}$ and $m^{(a)}(t) = G(t)^{-T}m^{(a)}$ the crystallographic directions transported to the configuration at time t , and (iv) the derivation of the basic kinematical relations by letting τ approach t .

We believe that the analysis of multiple slip in single crystals in this paper clarifies basic aspects of standard treatments that we describe now in more detail. Continuum studies from the 1960’s through the 1980’s (see Bassani, 1993 and Havner, 1992 for extensive references) have led to a well-established

framework for analyzing multiple slip in a variety of metallic single crystals. Central to the kinematics of multiple slip within this framework are two assumptions (see Bassani,1993 and Asaro,1983):

1. the macroscopic deformation gradient F can be factored $F = F^e F^p$ into an elastic part F^e and a plastic part F^p , in which F^p is intended to represent residual deformation after a material element is unloaded elastically, and F^e is intended to represent stretching and rotation of the crystalline lattice;
2. the rate of change of residual deformation relative to the lattice after slip is given by

$$\dot{F}^p F^{p-1} = \sum_{a=1}^A \dot{\gamma}^{(a)} s^{(a)} \otimes m^{(a)} \quad (1)$$

in which $\dot{\gamma}^{(a)}$ is intended to represent the slipping rate of the a^{th} -slip system, $s^{(a)}$ is a unit vector in the crystallographic direction in the reference configuration associated with the slip, and $m^{(a)}$ is the normal to the crystallographic plane in the reference configuration associated with the slip.

The above-mentioned framework for crystalline plasticity has led to successful calculations of geometrical changes and forces in single crystals that provide a practical justification for the framework. Nevertheless, the two assumptions above are difficult to understand and explain in their own right, because they contain a number of primitive quantities F^e , F^p , $\dot{\gamma}^{(a)}$ along with assumptions about their interrelation, leading to a variety of questions. What

is the mathematical definition of the quantity $\gamma^{(a)}$ whose time derivative is denoted by $\dot{\gamma}^{(a)}$? Why should the specific relation (1) rather than some variant be assumed? Why is the virtual, intermediate configuration associated with F^p needed at all? Why should (1) be the principal relation defining incremental slip in a single crystal? Although one can give plausible responses to these questions and can motivate by physical arguments the choices made in the above framework, one is left with a phenomenological theory in which the terminology, itself, is the principal guide to the user and the practical successes of the resulting theory compensate for these lingering questions.

In addition to deriving basic kinematical relations, in this paper we do obtain multiplicative decompositions $F = GM_r = M_lG$ for the macroscopic deformation gradient F in which each of the factors G , M_r , and M_l is identified in terms of limits of approximating piecewise-smooth mappings that reveal geometrical changes at a smaller length scale and that fix the transformation properties of each factor under change of observer and reference configuration. Although these multiplicative decompositions are not basic to our analysis of slip, the form of the relation $F = GM_r$ and the fact that G is the deformation due to smooth changes at smaller length scales do suggest an analogy with the standard relation $F = F^e F^p$. This analogy is further strengthened by comparison of the form of our derived relation (see eqn(50))

$$\dot{M}_r M_r^{-1} = \sum_{a=1}^A \lambda^{(a)} s^{(a)} \otimes m^{(a)} \quad (2)$$

with the form of the eqn(1) assumed in standard treatments. Nevertheless, we

approach this analogy cautiously, because in our relation $F = GM_r$, all of the quantities have been identified in a rigorous way and are purely geometrical, whereas in the relation $F = F^e F^p$ the quantities F^e and F^p are described informally and invoke the concepts of reversible loading and unloading as well as irreversible slips and, hence, are not purely geometrical.

2 Invertible Structured Deformations

We recall briefly (Del Piero & Owen, 1993) that specifying a structured deformation requires giving a piecewise smooth, injective mapping g that represents the macroscopic deformation of a body, as well as giving a piecewise continuous tensor field G that satisfies for some positive number m the inequalities

$$m \leq \det G(X) \leq \det \nabla g(X) \quad (3)$$

at every point X in the reference configuration \mathcal{A} . The Approximation Theorem (Del Piero & Owen, 1993) then assures that there exists a sequence $n \mapsto f_n$ of piecewise smooth, injective mappings (a *determining sequence* for g and G) satisfying

$$g = \lim_{n \rightarrow \infty} f_n \text{ and } G = \lim_{n \rightarrow \infty} \nabla f_n, \quad (4)$$

with the precise sense of convergence not relevant to the present discussion. Moreover, for every determining sequence, the following “identification rela-

tions” can be proven (Del Piero & Owen, 1993,1995):

$$M(X) := \nabla g(X) - G(X) = \lim_{r \rightarrow 0} \lim_{n \rightarrow \infty} \frac{\int_{\Gamma(f_n) \cap \mathcal{B}(X,r)} [f_n](Y) \otimes \nu(Y) dA_Y}{\text{vol}\mathcal{B}(X,r)} \quad (5)$$

$$G(X) = \lim_{r \rightarrow 0} \lim_{n \rightarrow \infty} \frac{\int_{\mathcal{B}} (X,r) \nabla f_n(Y) dV_Y}{\text{vol}\mathcal{B}(X,r)}. \quad (6)$$

Here, $\mathcal{B}(X,r)$ denotes the open ball centered at X of radius r , $\text{vol}\mathcal{B}(X,r)$ is its volume, $\Gamma(f_n)$ is the set on which f_n has jumps, $[f_n](Y)$ is the jump of f_n at the point $Y \in \Gamma(f_n)$, and $\nu(Y)$ is a unit normal to $\Gamma(f_n)$ at Y . The relation (5) shows that $M(X)$ is a double limit of surface integrals of the jumps in approximating deformations and permits us to identify $M(X)$ as the *deformation due to disarrangements* (Owen, 1995). In (6), $G(X)$ is computed as a double limit of volume averages of deformation gradients of approximating deformations, and we thus are justified calling $G(X)$ the *deformation without disarrangements*. In view of the identification relations (5) and (6), the simple formula

$$\nabla g(X) = G(X) + (\nabla g(X) - G(X)) = G(X) + M(X) \quad (7)$$

becomes a rigorously derived, *additive decomposition of the macroscopic deformation into the deformation without disarrangements $G(X)$ reflecting smooth geometrical changes at a smaller length scale, and the deformation due to disarrangements $M(X)$, reflecting non-smooth geometrical changes at a smaller length scale*. Moreover, each term f_n of a determining sequence $n \mapsto f_n$ for a given structured deformation permits us to view the body as breaking up into small pieces, each of which deforms smoothly and slides against

or separates from adjacent pieces, without interpenetration. As the index n increases, the number of pieces usually increases and their size decreases. The fields g and G required to specify a structured deformation are, in many important applications, actually smooth; nevertheless, the Approximation Theorem provides non-smooth deformations f_n , waiting in the wings to be used as needed, that reflect in detail the complicated geometrical changes occurring at smaller length scales.

To illustrate an application of identification relations, we note that relation (6) and known transformation properties for deformation gradients under change of observer or under change of reference configuration tell us that G , as a limit of averages of deformation gradients, transforms in the same way as ∇g ; the definition $M := \nabla g - G$ then tells us that M also transforms in the same way as ∇g . In addition the identification relation eqn(6) permits us to interpret the second inequality $\det G(X) \leq \det \nabla g(X)$ in eqn(3): the change in volume without disarrangements does not exceed the macroscopic change in volume. For the present study of deformations of single crystals, it is appropriate to assume that disarrangements are associated only with slip and, hence, cause no change in volume. Accordingly, we consider the following strengthening of the second inequality in eqn(3):

$$\det G(X) = \det \nabla g(X). \quad (8)$$

Following (Del Piero & Owen, 1993) , we call a structured deformation (g, G) satisfying eqn(8) at every point X an *invertible structured deformation*, and

we denote the set of invertible structured deformations (g, G) from a given reference configuration \mathcal{A} by $InvStd(\mathcal{A})$.

An immediate issue that can be clarified in the setting of (not necessarily invertible) structured deformations is that of multiplicative decompositions of the deformation gradient $F := \nabla g$. We recall that the additive decomposition eqn(7) is a mathematical consequence of the definition of structured deformations. We observe now that the additive decomposition immediately implies the following multiplicative decompositions of F :

$$F = G + M = G(I + G^{-1}M) = (I + MG^{-1})G. \quad (9)$$

Following (Del Piero & Owen, 1993) , we put

$$M_r := I + G^{-1}M, \quad (10)$$

$$M_l := I + MG^{-1}, \quad (11)$$

and we have:

$$F = GM_r = M_lG. \quad (12)$$

Going beyond the analysis in (Del Piero & Owen, 1993) , we note that substitution of the the identification relation eqn(5) for M into the formulas defining M_r and M_l provides the new identification relations

$$M_r(X) = I + \lim_{r \rightarrow 0} \lim_{n \rightarrow \infty} \frac{\int_{\Gamma(f_n) \cap \mathcal{B}(X, r)} G(X)^{-1} [f_n](Y) \otimes \nu(Y) dA_Y}{vol\mathcal{B}(X, r)}, \quad (13)$$

$$M_l(X) = I + \lim_{r \rightarrow 0} \lim_{n \rightarrow \infty} \frac{\int_{\Gamma(f_n) \cap \mathcal{B}(X, r)} [f_n](Y) \otimes G(X)^{-T} \nu(Y) dA_Y}{vol\mathcal{B}(X, r)}. \quad (14)$$

These relations show that both $M_r(X)$ and $M_l(X)$ equal the identity I if there are no jumps in the approximating deformations f_n . Moreover, because the jump in position $[f_n](Y)$ represents a vector determined by points in the deformed configuration of the body, the factor $G(X)^{-1}[f_n](Y)$ in the identification relation eqn(13) for $M_r(X)$ may be interpreted as a “pull-back” of the jump $[f_n](Y)$ by the deformation without disarrangements $G(X)$. Hence, $M_r(X)$ *measures the deformation due to disarrangements, pulling back the jumps via the deformation without disarrangements*. Similarly, the identification relation eqn(14) for $M_l(X)$ contains the factor $G(X)^{-T}\nu(Y)$ which may be interpreted as a “push-forward” of the normal $\nu(Y)$ in the reference configuration by the deformation without disarrangements. Hence, $M_l(X)$ *measures the deformation due to disarrangements, pushing forward the normals to jump surfaces in the reference configuration via the deformation without disarrangements*.

It is important to remember that M_r , M_l , and M are measures of the effect at the macrolevel of non-smooth deformations at a smaller length scale in the precise sense given in the identification relations eqn(13), (14), and (5). As such, these tensors are purely geometrical quantities and, in the present context, do not carry the attributes of reversibility or irreversibility. Only with the prescription of constitutive relations would reversibility and irreversibility become meaningful.

As we remarked above, M and G transform in the same way as F under change in observer and change in reference configuration. This observation,

together with eqns(10) and (11), yields the following list of transformation laws:

Changeofobserver	Changeofreferenceconfiguration
$F \rightarrow QF$	$F \rightarrow FH$
$G \rightarrow QG$	$G \rightarrow GH$
$M \rightarrow QM$	$M \rightarrow MH$
$M_r \rightarrow M_r$	$M_r \rightarrow H^{-1}M_rH$
$M_l \rightarrow QM_lQ^T$	$M_l \rightarrow M_l$

We note also the identification relation for $tr(M(X)G(X)^{-1})$ that follows from eqns(10) and (13):

$$\begin{aligned}
tr(M(X)G(X)^{-1}) &= tr(M_r(X) - I) = tr(M_l(X) - I) \\
&= \lim_{r \rightarrow 0} \lim_{n \rightarrow \infty} \frac{\int_{\Gamma(f_n) \cap \mathcal{B}(X,r)} G(X)^{-1}[f_n](Y) \cdot \nu(Y) dA_Y}{vol\mathcal{B}(X,r)} \quad (15)
\end{aligned}$$

Consequently, the vanishing of $tr(M(X)G(X)^{-1})$ for a given structured deformation indicates through this relation that, on average, the deformations due to disarrangements arise through tangential jumps. We denote by $\{G(X)^{-T}\}^\perp$ the subspace of $Lin\mathcal{V}$ consisting of all tensors $U \in Lin\mathcal{V}$ satisfying

$$U \cdot G(X)^{-T} := tr(UG(X)^{-1}) = 0. \quad (16)$$

We denote by $M^0(X)$ the tensor in the subspace $\{G(X)^{-T}\}^\perp$ that is closest to the disarrangement tensor $M(X) = \nabla g(X) - G(X)$ and note that

$$M^0(X) = M(X) - \frac{M(X) \cdot G(X)^{-T}}{|G(X)^{-T}|^2} G(X)^{-T}. \quad (17)$$

3 Approximations of disarrangements

We consider in this section an invertible structured deformation $(g, G) \in \text{InvStd}(\mathcal{A})$, a point $X \in \mathcal{A}$. The following estimate is the starting point for our subsequent approximations of disarrangements by slips:

$$\begin{aligned} & \left| M(X) - M^0(X) \right| \leq \\ & \left(2 \left| G(X)^{-T} \right| + |M(X)| \left| G(X)^{-T} \right|^{-1} \det G(X)^{-1} \right) |M(X)|^2. \end{aligned} \quad (18)$$

This estimate provides a bound for the distance from $M(X)$ to the given subspace $\{G(X)^{-T}\}^\perp$ that goes to zero with the square of the norm of $M(X)$. This bound is valid even for large disarrangements, but it provides accurate approximations as disarrangements become small.

In the following verification of eqn(18), we omit the dependence of tensors on X . Because the tensor G^{-T} is orthogonal to every tensor in the subspace $\{G^{-T}\}^\perp$, the distance from the tensor M to $\{G^{-T}\}^\perp$ is given by the formula

$$\left| M - M^0 \right| = \frac{|M \cdot G^{-T}|}{|G^{-T}|} = \frac{|tr(MG^{-1})|}{|G^{-T}|}. \quad (19)$$

However, eqns(8) and (9) yield

$$\begin{aligned} 1 &= \det(MG^{-1} + I) \\ &= 1 + tr(MG^{-1}) + \frac{1}{2}(tr(MG^{-1}))^2 - \frac{1}{2}tr((MG^{-1})^2) + \det M \det G^{-1} \end{aligned}$$

so that

$$tr(MG^{-1}) = -\frac{1}{2}(tr(MG^{-1}))^2 + \frac{1}{2}tr((MG^{-1})^2) - \det M \det G^{-1}. \quad (20)$$

Writing the first two terms on the right-hand side in terms of inner products of tensors yields the estimates

$$(tr(MG^{-1}))^2 \leq |M|^2 |G^{-T}|^2,$$

$$|tr((MG^{-1})^2)| = |(MG^{-1})^2 \cdot I| \leq |MG^{-1}|^2 |I| \leq 3 |M|^2 |G^{-T}|^2,$$

and elementary properties of the determinant yield the inequality $|\det M| \leq |M|^3$. These inequalities and eqn(20) yield the estimate

$$|tr(MG^{-1})| \leq \left(2 |G^{-T}|^2 + |M| |\det G^{-1}|\right) |M|^2$$

which, together with eqn(19) establishes eqn(18).

The fact that the coefficient $2 |G^{-T}| + |M| |G^{-T}|^{-1} |\det G^{-1}|$ of $|M|^2$ in eqn(18) depends continuously upon G and M implies that *there exist positive numbers k^0 and η^0 such that for each $(g, G) \in InvStd(\mathcal{A})$ and $X \in \mathcal{A}$:*

$$|M(X) - M^0(X)| \leq k^0 |M(X)|^2 \tag{21}$$

whenever $|G(X) - I|$ and $|M(X)|$ are less than η^0 .

4 Slip-approximations for deformations of single crystals

A description of the deformation due to disarrangements that can occur in a given continuum must take into account observed restrictions at sub-macroscopic length scales on the directions of the disarrangements and on the orientation of the disarrangement sites. These restrictions on sub-macroscopic

geometrical changes are included within the present geometrical setting through the choice of a subspace of $\{G(X)^{-T}\}^\perp$ that provides an exact description of the restrictions. In this section we give an approximation to the deformation due to disarrangements $M(X)$ that lies in the identified subspace, and we provide error-bounds that decrease with the square of the norm of $M(X)$.

For a crystal in the reference configuration \mathcal{A} the crystallographic data required for our analysis of multiple slip consists of pairs of orthogonal unit vectors $s^{(a)}, m^{(a)}$, $a = 1, \dots, A$, with A the number of potentially active slip systems. The vector $s^{(a)}$ is the direction of slip, and the vector $m^{(a)}$ is the normal to the slip plane for the a^{th} slip-system (Asaro, 1983). These data and the deformation without disarrangements $G(X)$ determine the subspace of $\text{Lin}\mathcal{V}$

$$\mathcal{C}(G(X)) := \text{Lsp} \left\{ G(X)s^{(a)} \otimes m^{(a)} \mid a = 1, \dots, A \right\} \quad (22)$$

In fact, $\mathcal{C}(G(X))$ is a subspace of $\{G(X)^{-T}\}^\perp$, because

$$\begin{aligned} (G(X)s^{(a)} \otimes m^{(a)}) \cdot G(X)^{-T} &= \text{tr}(G(X)s^{(a)} \otimes m^{(a)}G(X)^{-1}) \\ &= \text{tr}(s^{(a)} \otimes m^{(a)}) = 0. \end{aligned}$$

We denote by $M_{\mathcal{C}(G(X))}$ the tensor in $\mathcal{C}(G(X))$ that is closest to the disarrangement tensor $M(X)$, and we observe that, when $\mathcal{C}(G(X))$ is a proper subspace of $\{G(X)^{-T}\}^\perp$, the tensor $M_{\mathcal{C}(G(X))}$ may be different from the tensor $M^0(X)$. In any case, we may conclude from eqn(17) and the fact that both $M_{\mathcal{C}(G(X))}$ and $M^0(X)$ are in $\{G(X)^{-T}\}^\perp$:

$$\left| M(X) - M_{\mathcal{C}(G(X))} \right|^2 = \left| M(X) - M^0(X) \right|^2 + \left| M^0(X) - M_{\mathcal{C}(G(X))} \right|^2. \quad (23)$$

Although for each invertible structured deformation the quantity $|M(X) - M^0(X)|$ on the right-hand side of eqn(23) obeys the inequality eq(21), there does not appear to be a corresponding estimate for the quantity $|M^0(X) - M_{\mathcal{C}(G(X))}|$ valid for arbitrary invertible structured deformations. We note that $M_{\mathcal{C}(G(X))}$ is a finite sum of scalar multiples of the diads $G(X)s^{(a)} \otimes m^{(a)}$ and that each disarrangement tensor is approximated via the identification relation eqn(5) by an integral of diads $[f_n](Y) \otimes \nu(Y)$. Accordingly, we interpret the number $|M^0(X) - M_{\mathcal{C}(G(X))}|$ as arising from the replacement of a limit of integrals — in whose integrands the directions of jumps $[f_n](Y)$ need not be in “updated” crystallographic directions $G(X)s^{(a)}$ and in which the normals $\nu(Y)$ need not be one of the crystallographic normals $m^{(a)}$ — by a linear combination of the crystallographic diads.

We now identify a collection of invertible structured deformations for which the differences $|M^0(X) - M_{\mathcal{C}(G(X))}|$ do satisfy an estimate of the form eq(21). Specifically, for given crystallographic data $s^{(a)}, m^{(a)}$, $a = 1, \dots, A$, we denote by $Crys(\mathcal{A})$ the set of all invertible structured deformations $(g, G) \in InvStd(\mathcal{A})$ such that for every $X \in \mathcal{A}$:

$$|M^0(X) - M_{\mathcal{C}(G(X))}| \leq k^0 |M(X)|^2 \quad (24)$$

whenever $|G(X) - I|$ and $|M(X)|$ are less than η^0 , with $k^0 > 0$ and $\eta^0 > 0$ the numbers identified above eqn(21). We note that the set $Crys(\mathcal{A})$ contains all structured deformations in which g is a homogeneous deformation, G is a

constant, and $M = \nabla g - G$ is a constant of the form

$$M = \sum_{a=1}^A \beta^{(a)} G s^{(a)} \otimes m^{(a)} + \alpha G^{-T}, \quad (25)$$

where the only restriction on the numbers $\beta^{(a)}$ and α is imposed by the relation $\det(G + M) = \det G$. In this example, $M^0(X) = M_{\mathcal{C}(G(X))} = \sum_{a=1}^A \beta^{(a)} G s^{(a)} \otimes m^{(a)}$.

Our main result on multiple slip follows immediately from eqns(21), (23), and (24) and gives an estimate for the difference between $M(X)$ and an appropriate combination of crystallographic diads $G(X)s^{(a)} \otimes m^{(a)}$: *there exist positive numbers k and η such that, for each $X \in \mathcal{A}$ and each invertible structured deformation $(g, G) \in \text{Crys}(\mathcal{A})$, there are numbers $\delta^{(a)}(X)$, $a \in \{1, \dots, A\}$ for which*

$$\left| M(X) - \sum_{a=1}^A \delta^{(a)}(X) G(X) s^{(a)} \otimes m^{(a)} \right| \leq k |M(X)|^2 \quad (26)$$

whenever $|G(X) - I|$ and $|M(X)|$ are less than η .

We call the tensor $\sum_{a=1}^A \delta^{(a)}(X) G(X) s^{(a)} \otimes m^{(a)}$ in eqn(26) a *slip-approximation* of $M(X)$ for the given single crystal. In the analysis above, we have the formula $\sum_{a=1}^A \delta^{(a)}(X) G(X) s^{(a)} \otimes m^{(a)} = M_{\mathcal{C}(G(X))}$, with $M_{\mathcal{C}(G(X))}$ the element of $\mathcal{C}(G(X))$ closest to $M(X)$. However, the numbers $\delta^{(a)}(X)$, $a \in \{1, \dots, A\}$, in general, are not uniquely determined by this formula. If the set of diads $\{G(X)s^{(a)} \otimes m^{(a)} \mid a = 1, \dots, A\}$ is a linearly independent subset of $\text{Lin}\mathcal{V}$, so that it is a basis of $\mathcal{C}(G(X))$, then $\delta^{(a)}(X)$, $a \in \{1, \dots, A\}$ are uniquely determined. In any case, we call $\delta^{(a)}(X)$ the *shear in the a^{th} slip-system*

for the slip-approximation $\sum_{a=1}^A \delta^{(a)}(X)G(X)s^{(a)} \otimes m^{(a)}$ to $M(X)$. Even when this set of diads is linearly dependent, the inequality eqn(26) tells us that, *as the deformation without disarrangements $M(X)$ tends to zero, the slip-approximation $\sum_{a=1}^A \delta^{(a)}(X)G(X)s^{(a)} \otimes m^{(a)}$ converges quadratically to $M(X)$.*

We note that the approximation $\sum_{a=1}^A \delta^{(a)}(X)G(X)s^{(a)} \otimes m^{(a)}$ for $M(X)$ yields immediately the following inequalities and approximations for the tensors $M_r(X)$ and $M_l(X)$ defined in eqns(10),(11):

$$\left| M_r(X) - \left(I + \sum_{a=1}^A \delta^{(a)}(X)s^{(a)} \otimes m^{(a)} \right) \right| \leq c |M(X)|^2, \quad (27)$$

$$\left| M_l(X) - \left(I + \sum_{a=1}^A \delta^{(a)}(X)G(X)s^{(a)} \otimes G(X)^{-T}m^{(a)} \right) \right| \leq c |M(X)|^2, \quad (28)$$

where the positive number c depends upon $G(X)$ in an explicit manner that we do not record here. We note that the approximations $\sum_{a=1}^A \delta^{(a)}(X)G(X)s^{(a)} \otimes m^{(a)}$, $I + \sum_{a=1}^A \delta^{(a)}(X)s^{(a)} \otimes m^{(a)}$, and $I + \sum_{a=1}^A \delta^{(a)}(X)G(X)s^{(a)} \otimes G(X)^{-T}m^{(a)}$ transform under changes of observer and of reference configuration in the same manner as the tensors $M(X)$, $M_r(X)$, and $M_l(X)$, respectively.

5 Time-parameterized families of invertible structured deformations

In order to follow the deformation of a body in time, we consider a time-interval \mathcal{I} and assume for each time $\tau \in \mathcal{I}$ there is given an invertible structured deformation $(g(\cdot, \tau), G(\cdot, \tau)) \in \text{InvStd}(\mathcal{A})$. We denote by $F(\cdot, \tau)$,

$G(\cdot, \tau), M(\cdot, \tau), M_r(\cdot, \tau)$ and $M_l(\cdot, \tau)$ the fields on \mathcal{A} at time τ that correspond to F, G, M, M_r, M_l introduced above. In particular, the fields at time τ obey additive and multiplicative decompositions as well as identification relations corresponding to those in Section 2.

In order to describe *structured deformations relative to the configuration* $\mathcal{A}(t)$ occupied by the body at time $t \in \mathcal{I}$, we define for each $x \in \mathcal{A}(t)$ and $\tau \in \mathcal{I}$

$$g_t(x, \tau) := g(X, \tau) \text{ and } G_t(x, \tau) := G(X, \tau)G(X, t)^{-1}, \quad (29)$$

where $X \in \mathcal{A}$ is determined by the relation $x = g(X, t)$, so that $X = g(\cdot, t)^{-1}(x)$. It can be shown that $(g_t(\cdot, \tau), G_t(\cdot, \tau))$ is an invertible structured deformation from $\mathcal{A}(t)$, and we may consider the fields $F_t(\cdot, \tau) := \nabla g_t(\cdot, \tau)$, $G_t(\cdot, \tau)$, and $M_t(\cdot, \tau)$ describing, respectively, the (macroscopic) deformation gradient, the deformation without disarrangements, and the deformation due to disarrangements at time τ , each relative to the configuration at time t . The additive decomposition of deformation gradient eqn(7) and the identification relation eqn(5) become in this context

$$F_t(x, \tau) = G_t(x, \tau) + M_t(x, \tau) \quad (30)$$

$$M_t(x, \tau) := F_t(x, \tau) - G_t(x, \tau) = \lim_{r \rightarrow 0} \lim_{n \rightarrow \infty} \frac{\int_{\Gamma_t(f_n(\cdot, \tau)) \cap \mathcal{B}(x, r)} [f_n](y, \tau) \otimes \nu(y, \tau) dA_y}{\text{vol} \mathcal{B}(x, r)}, \quad (31)$$

now with $n \mapsto f_n(\cdot, \tau)$ a determining sequence for the invertible structured deformation $(g_t(\cdot, \tau), G_t(\cdot, \tau))$, with $\Gamma_t(f_n(\cdot, \tau))$ the set of jump points of the n^{th} -term $f_n(\cdot, \tau)$, with $\nu(y, \tau)$ a unit normal to $\Gamma_t(f_n(\cdot, \tau))$ at $y \in \Gamma_t(f_n(\cdot, \tau)) \cap$

$\mathcal{B}(x, r)$, and with $\mathcal{B}(x, r) \subset \mathcal{A}(t)$ the open ball of radius r centered at the point $x \in \mathcal{A}(t)$.

In order to introduce various rates of deformation relative to the configuration at time t , we note the relation

$$F_t(x, \tau) = F(X, \tau)F(X, t)^{-1}, \quad X = g(\cdot, t)^{-1}(x) \quad (32)$$

among the relative deformation gradient and the deformation gradients at times τ and t . In addition to the smoothness tacit in the assumption $(g(\cdot, \tau), G(\cdot, \tau)) \in \text{InvStd}(\mathcal{A})$ for each $\tau \in \mathcal{I}$, we assume that $F(X, \cdot)$ and $G(X, \cdot)$ are differentiable, and eqns(32), (29), and (30) then imply that $F_t(x, \cdot)$, $G_t(x, \cdot)$, and $M_t(x, \cdot)$ not only are differentiable but also satisfy the relation

$$\frac{\partial}{\partial \tau} F_t(x, \tau) = \frac{\partial}{\partial \tau} G_t(x, \tau) + \frac{\partial}{\partial \tau} M_t(x, \tau) \quad (33)$$

for every $t, \tau \in \mathcal{I}$.

For each $X \in \mathcal{A}$ and $t \in \mathcal{I}$ we define relative rates of deformation $L(X, t)$, $L_G(X, t)$, and $L_M(X, t)$ through the relations

$$L(X, t) := \frac{\partial}{\partial \tau} F_t(g(X, t), \tau) \Big|_{\tau=t}, \quad (34)$$

$$L_G(X, t) := \frac{\partial}{\partial \tau} G_t(g(X, t), \tau) \Big|_{\tau=t}, \quad (35)$$

$$L_M(X, t) := \frac{\partial}{\partial \tau} M_t(g(X, t), \tau) \Big|_{\tau=t}. \quad (36)$$

While $L(X, t)$ is the standard measure of rate of deformation relative to the configuration at time t , the rates $L_G(X, t)$ and $L_M(X, t)$ are introduced here by analogy to the standard one. We call $L_G(X, t)$ the *relative rate*

of deformation without disarrangements and $L_M(X, t)$ the relative rate of deformation due to disarrangements. We deduce immediately from eqns(29), (32), and (33) the formulae

$$L(X, t) = \dot{F}(X, t)F(X, t)^{-1}, \quad (37)$$

$$L_G(X, t) = \dot{G}(X, t)G(X, t)^{-1}, \quad (38)$$

and

$$L(X, t) = L_G(X, t) + L_M(X, t), \quad (39)$$

so that the relative rate of deformation is the sum of the relative rate of deformation without disarrangements and the relative rate of deformation due to disarrangements. We note that these rates of deformation are purely kinematical quantities that, in the present discussion without specified constitutive relations, carry no attributes of reversibility or irreversibility.

The relations $M_r(X, t) = G(X, t)^{-1}F(X, t)$ and $M_l(X, t) = F(X, t)G(X, t)^{-1}$ in eqn(12) together with eqns(37)-(39) yield after some computation

$$\dot{M}_r(X, t)M_r(X, t)^{-1} = G(X, t)^{-1}L_M(X, t)G(X, t) \quad (40)$$

and

$$\dot{M}_l(X, t)M_l(X, t)^{-1} = L(X, t) - M_l(X, t)L_G(X, t)M_l(X, t)^{-1}. \quad (41)$$

The transformation properties of the kinematical quantities introduced in this section under time-dependent changes in observer and under changes of

reference configuration follow easily from the relations above, and we record them in the following tables:

Changeofobserver

$$\begin{aligned}
F(X, t) &\rightarrow Q(X, t)F(X, t) \\
G(X, t) &\rightarrow Q(X, t)G(X, t) \\
M(X, t) &\rightarrow Q(X, t)M(X, t) \\
L(X, t) &\rightarrow \dot{Q}(X, t)Q(X, t)^T + Q(X, t)L(X, t)Q(X, t)^T \\
L_G(X, t) &\rightarrow \dot{Q}(X, t)Q(X, t)^T + Q(X, t)L_G(X, t)Q(X, t)^T \\
L_M(X, t) &\rightarrow Q(X, t)L_M(X, t)Q(X, t)^T \\
\dot{M}_r(X, t)M_r(X, t)^{-1} &\rightarrow \dot{M}_r(X, t)M_r(X, t)^{-1}
\end{aligned}$$

Changeofreferenceconfiguration

$$\begin{aligned}
F(X, t) &\rightarrow F(X, t)H \\
G(X, t) &\rightarrow G(X, t)H \\
M(X, t) &\rightarrow M(X, t)H \\
L(X, t) &\rightarrow L(X, t) \\
L_G(X, t) &\rightarrow L_G(X, t) \\
L_M(X, t) &\rightarrow L_M(X, t). \\
\dot{M}_r(X, t)M_r(X, t)^{-1} &\rightarrow H^{-1}\dot{M}_r(X, t)M_r(X, t)^{-1}H
\end{aligned}$$

It is interesting to note that, while L and L_{Grm} do not transform objectively under change of observer, *the relative rate of deformation due to disarrangements* L_M *does transform objectively.*

We also note for future reference the relations

$$F_t(x, t) = G_t(x, t) = I, \quad M_t(x, t) = 0, \quad tr L_M(X, t) = 0. \quad (42)$$

6 Representations for incremental slip in single crystals

The analysis that we undertake in this section is intended to describe the geometrical changes that result at each time τ due to (relative) invertible

structured deformations $(g_t(\cdot, \tau), G_t(\cdot, \tau)) \in \text{InvStd}(\mathcal{A}(t))$ from a point $x = g(X, t)$ in the current configuration. The approximations derived in Section 4 are well-suited for the present purpose. To employ them, we replace the fixed reference configuration \mathcal{A} employed in Sections 3 and 4 by the current configuration $\mathcal{A}(t)$, and we replace the crystallographic pairs $s^{(a)}, m^{(a)}$, $a = 1, \dots, A$, associated with \mathcal{A} by the pairs of orthogonal (but not necessarily unit) vectors $s^{(a)}(x, t), m^{(a)}(x, t)$ defined by

$$s^{(a)}(x, t) := G(X, t)s^{(a)}, \quad m^{(a)}(x, t) := G(X, t)^{-T}m^{(a)}, \quad a = 1, \dots, A, \quad (43)$$

obtained via the invertible structured deformation $(g(\cdot, t), G(\cdot, t)) \in \text{InvStd}(\mathcal{A})$, with $x = g(X, t)$ as above. (The latter pairs of vectors reflect the effects of the distortion of the crystalline lattice, measured here by the deformation without disarrangements $G(\cdot, t)$.) Finally, we replace $G(X)$ by $G_t(x, \tau)$ in the definition of the subspace $\mathcal{C}(G(X))$ in eqn(22) and in the formula eqn(17), yielding the tensor $M_t^0(x, \tau)$ in the subspace $\{G_t(x, \tau)^{-T}\}^\perp$ that is closest to the relative disarrangement tensor $M_t(x, \tau) = \nabla g_t(x, \tau) - G_t(x, \tau)$ in eqn(31).

Let $t \in \mathcal{I}$ and $x \in \mathcal{A}(t)$ be given, and assume that there is an open interval $\mathcal{J}(t) \subset \mathcal{I}$ such that for every $\tau \in \mathcal{J}(t)$, $(g_t(\cdot, \tau), G_t(\cdot, \tau)) \in \text{Crys}(\mathcal{A}(t))$. This assumption implies that the inequality eqn(26) has the following counterpart: *there are positive numbers $k(x, t)$ and $\eta(x, t)$ such that, for every $\tau \in \mathcal{J}(t)$, there exist numbers $\delta_t^{(a)}(x, \tau)$, $a \in \{1, \dots, A\}$ for which*

$$\left| M_t(x, \tau) - \sum_{a=1}^A \delta_t^{(a)}(x, \tau) G_t(x, \tau) s^{(a)}(x, t) \otimes m^{(a)}(x, t) \right| \leq k(x, t) |M_t(x, \tau)|^2 \quad (44)$$

whenever $|G_t(x, \tau) - I|$ and $|M_t(x, \tau)|$ are less than $\eta(x, t)$. We remark that, by eqn(42) and the smoothness of $G_t(x, \cdot)$ and $M_t(x, \cdot)$, the numbers $|G_t(x, \tau) - I|$ and $|M_t(x, \tau)|$ tend to zero as τ tends to t , so that eqn(44) is satisfied for $|\tau - t|$ sufficiently small. Moreover, the collection $Crys(\mathcal{A}(t))$ now depends upon x as well as upon t through the crystallographic diads $s^{(a)}(x, t) \otimes m^{(a)}(x, t)$, and we indicate this dependence through the notation $Crys_x(\mathcal{A}(t))$.

We now divide the members of eqn(44) by $|\tau - t|$, we invoke the smoothness of the family $(g(\cdot, \tau), G(\cdot, \tau)) \in InvStd(\mathcal{A})$ together with eqns(42) and (36), and we let $\tau \rightarrow t$ to conclude that the ratio $\frac{\sum_{a=1}^A \delta_t^{(a)}(x, \tau) G_t(x, \tau) s^{(a)}(x, t) \otimes m^{(a)}(x, t)}{(\tau - t)}$ has a limit as τ tends to t and

$$L_M(X, t) = \lim_{\tau \rightarrow t} \frac{\sum_{a=1}^A \delta_t^{(a)}(x, \tau) G_t(x, \tau) s^{(a)}(x, t) \otimes m^{(a)}(x, t)}{\tau - t}, \quad (45)$$

i.e., the relative rate of deformation due to disarrangements for the given family of invertible structured deformations equals the limit of the quotient

$$Q_t(x, \tau) := \sum_{a=1}^A \delta_t^{(a)}(x, \tau) G_t(x, \tau) s^{(a)}(x, t) \otimes m^{(a)}(x, t) / (\tau - t)$$

as τ tends to t . Thus, the error in the approximations $Q_t(x, \tau)$ to $M_t(x, \tau) / (\tau - t)$ vanishes in the limit as τ tends to t . We note that $L_M(X, t)$ is traceless, by eqn(33), but that the quotients $Q_t(x, \tau)$ need not be. Following the terminology in Section 4, we call the tensor $\sum_{a=1}^A \delta_t^{(a)}(x, \tau) G_t(x, \tau) s^{(a)}(x, t) \otimes m^{(a)}(x, t)$ a *slip-approximation to the relative disarrangement tensor* $M_t(x, \tau)$, and we call the number $\delta_t^{(a)}(x, \tau)$ the *relative shear in the a^{th} slip-system* for the slip-approximation.

The representation formula eqn(45) can be simplified further by writing

$$\begin{aligned} L_M(X, t) &= \lim_{\tau \rightarrow t} \sum_{a=1}^A \frac{\delta_t^{(a)}(x, \tau)}{\tau - t} G_t(x, \tau) s^{(a)}(x, t) \otimes m^{(a)}(x, t) \\ &= \lim_{\tau \rightarrow t} G_t(x, \tau) \sum_{a=1}^A \frac{\delta_t^{(a)}(x, \tau)}{\tau - t} s^{(a)}(x, t) \otimes m^{(a)}(x, t). \end{aligned} \quad (46)$$

Noting that $\lim_{\tau \rightarrow t} G_t(x, \tau) = I$ and, for each τ , the tensor $\sum_{a=1}^A \frac{\delta_t^{(a)}(x, \tau)}{\tau - t} s^{(a)}(x, t) \otimes m^{(a)}(x, t)$ is in the subspace $\mathcal{C}(G_t(x, \tau))|_{\tau=t}$, we conclude that

$$\begin{aligned} \sum_{a=1}^A \frac{\delta_t^{(a)}(x, \tau)}{\tau - t} s^{(a)}(x, t) \otimes m^{(a)}(x, t) = \\ G_t(x, \tau)^{-1} \left(G_t(x, \tau) \sum_{a=1}^A \frac{\delta_t^{(a)}(x, \tau)}{\tau - t} s^{(a)}(x, t) \otimes m^{(a)}(x, t) \right) \end{aligned}$$

has a limit as $\tau \rightarrow t$ that also lies in $\mathcal{C}(G_t(x, \tau))|_{\tau=t}$. Therefore, we may choose real numbers $\lambda^{(a)}(x, t)$, $a = 1, \dots, A$, such that

$$\lim_{\tau \rightarrow t} \sum_{a=1}^A \frac{\delta_t^{(a)}(x, \tau)}{\tau - t} s^{(a)}(x, t) \otimes m^{(a)}(x, t) = \sum_{a=1}^A \lambda^{(a)}(x, t) s^{(a)}(x, t) \otimes m^{(a)}(x, t),$$

and eqn(46) yields the following *slip-representation for the relative rate of deformation due to disarrangements*:

$$L_M(X, t) = \sum_{a=1}^A \lambda^{(a)}(x, t) s^{(a)}(x, t) \otimes m^{(a)}(x, t). \quad (47)$$

We observe that this purely kinematical relation is based on the geometry of structured deformations and on the derived representation eqn(45) for incremental disarrangements, without reference to constitutive relations. Nevertheless, our slip-representation is of the same form as the assumed formula for the “plastic part” of the velocity gradient in standard treatments of

crystalline plasticity (Asaro,1983, eqn(2.10)). From the outset, these treatments interpret plastic deformation as dissipative and, hence, tacitly entail constitutive assumptions. In spite of this difference, each number $\lambda^{(a)}(x, t)$ in our eqn(47) corresponds to the number $\dot{\gamma}^{(a)}$ in (Asaro, 1983), called there the “slipping rate of the a^{th} slip-system”. In our derivation of eq(47) above, the numbers $\lambda^{(a)}(x, t)$ arise through limits of sums of quotients in which the numerators contain the relative shears $\delta_t^{(a)}(x, \tau)$ for each slip system and the denominators are $\tau - t$. This fact supports the terminology chosen in standard treatments.

It should be noted that the diads $s^{(a)}(x, t) \otimes m^{(a)}(x, t)$, $a = 1, \dots, A$, generally are linearly dependent, and this dependence implies that the numbers $\lambda^{(a)}(x, t)$ are not uniquely determined by eqn(47). In the special case where the diads $s^{(a)}(x, t) \otimes m^{(a)}(x, t)$, $a = 1, \dots, A$, form a linearly independent subset of $Lin\mathcal{V}$, each quotient $\frac{\delta_t^{(a)}(x, \tau)}{\tau - t}$ will have a limit as $\tau \rightarrow t$, and the numbers $\lambda^{(a)}(x, t)$, $a = 1, \dots, A$, will be given by the formulas

$$\lambda^{(a)}(x, t) = \lim_{\tau \rightarrow t} \frac{\delta_t^{(a)}(x, \tau)}{\tau - t}, \quad a = 1, \dots, A. \quad (48)$$

Accordingly, we call the number $\lambda^{(a)}(x, t)$ the *relative shear rate for the a^{th} slip-system* (even in the case where the diads are linearly dependent).

Eqns(47), (39), and (38) now yield for the case of incremental slip the *decomposition of the relative rate of deformation into a part without disarrangements and a part due to disarrangements* :

$$L(X, t) = L_G(X, t) + L_M(X, t)$$

$$= \dot{G}(X, t)G(X, t)^{-1} + \sum_{a=1}^A \lambda^{(a)}(x, t)s^{(a)}(x, t) \otimes m^{(a)}(x, t) \quad (49)$$

with $x = g(X, t)$. In a similar way, eqns(39) and (40) yield in the case of incremental slip a formula for $\dot{M}_r M_r^{-1}$:

$$\begin{aligned} \dot{M}_r(X, t)M_r(X, t)^{-1} &= G(X, t)^{-1}L_M(X, t)G(X, t) \\ &= \sum_{a=1}^A \lambda^{(a)}(x, t)s^{(a)} \otimes m^{(a)} \end{aligned} \quad (50)$$

with $x = g(X, t)$. Keeping in mind the qualifications made earlier, we note the similarity of our derived formula for $\dot{M}_r M_r^{-1}$ and the one assumed for “ $\dot{F}^p F^{p-1}$ ” in standard presentations, e.g., below eq(2.10) in (Asaro,1983) and eqn(2.8) in (Bassani, 1993).

We remark that the analysis above can be carried out when the dependence upon τ of $M_t(x, \tau)$ and $G_t(x, \tau)$ is less smooth, provided only that there exist a sequence $n \mapsto \tau_n$ of times for which $M_t(x, \tau_n)/(\tau_n - t)$ has a limit, $M_t(x, \tau_n)$ tends to zero, and $G_t(x, \tau_n)$ is bounded as $\tau_n \rightarrow t$. This weaker smoothness hypothesis may be appropriate on time scales where slip occurs in small, discrete time-steps.

Acknowledgments: This research was supported by the National Science Foundation Grant DMS 9703863, by the Center for Nonlinear Analysis, Department of Mathematical Sciences of Carnegie Mellon University, and by the Italian M.U.R.S.T. through the grant “Modelli matematici per la scienza dei materiali”-Co.Fin. (1998).

7 References

- Asaro, R. J.(1983) Crystal plasticity, *J. Appl. Mechanics* **50**, 921-934.
- Bassani, J.L. (1993) Plastic flow of crystals. In *Advances in Applied Mechanics* **30**, ed. J. W. Hutchinson and T. Y. Wu, pp. 191-258.
- Del Piero, G. and Owen, D.R. (1993) Structured deformations of continua, *Arch. Rational Mech. Anal.* **124**, 99-155.
- Del Piero, G. and Owen, D.R. (1995) Integral-gradient formulae for structured deformations, *Arch. Rational Mech. Anal.* **131**, 121-138.
- Havner, K.S.(1992) *Finite Plastic Deformation of Crystalline Solids*. Cambridge Monographs in Mechanics and Applied Mathematics, Cambridge University Press, Cambridge.
- Owen, D.R. (1995) Disarrangements in continua and the geometry of microstructure. In *Recent Advances in Elasticity, Viscoelasticity and Inelasticity*, ed. K. Rajagopal, 67-81.