Material symmetry in a theory of continuously defective crystals

M. Elżanowski* and G. Parry (`gareth.parry@nottingham.ac.uk`)
School of Mathematical Sciences, University of Nottingham,
Pope Building, Nottingham NG7 2RD, England

Abstract. We propose that a particular group, which depends on the dislocation density tensor, be adopted as material symmetry group for some classes of defective crystals, and give motivation for this proposal.

1. Introduction

The motivation for this work is the desire to compare two different theories of defective crystals. The first theory was initiated by Davini[4] in 1986 – in that theory a crystal state is defined by the prescription of three smooth linearly independent lattice vector fields at each point of a domain $\Omega \subseteq \mathbb{R}^3$. The focus of that theory is on objects which are elastic invariants, like the Bürger's vector and the dislocation density tensor. Since elastic deformation does not change these objects, they measure inelastic (or 'plastic') changes. The theory has developed to the extent that there is a place in it for the analogue of kinematical mechanisms that appear in phenomenological plasticity theories, specifically changes of state which leave the elastic invariants unchanged, but which are not elastic, represent slip in planes (for example) where the lattice vector fields are constant. Davini and Parry [5],[6] call such changes neutral deformations, and note in particular that it is necessary that the dislocation density tensor be singular if neutral deformations are to exist. Some variational problems which allow both for slip and for elastic deformation have been studied, Davini and Parry [5],[6] and Fonseca and Parry [9], but there is no detailed model which accounts for the evolution of the elastic invariants, yet, in this theory.

The second theory is based on work by Noll [12] in the 1960s. There the central assumption is that a relevant strain energy density may be expressed as a function of deformation gradient (with respect to some reference state) and reference position. (In fact, the discussion is

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* Permanent address: Department of Mathematics and Statistics, Portland State University P O Box 751, Portland, OR 97207, USA

in terms of general 'response functions'). A first issue that is addressed is whether or not the given strain energy density represents a 'uniform material', where it is supposed that a material is uniform if there exists a reference configuration such that the strain energy density, expressed with respect to that reference configuration, is independent of position. So if a material is uniform, and a strain energy density with respect to some arbitrary reference configuration is given, then there is defined a generally non-integrable change of configuration (to the uniform one), and this can be thought of as prescribing a 'frame' (consisting of three linearly independent vector fields). The frame is determined only to within elements of the isotropy group of the strain energy density, which adds complexity. However, the existence of a frame provides an apparent point of contact between the two theories, and indeed there is a correspondence between one of the main objects of this geometrical theory, which is the torsion (of the connection defined by the frame), and the dislocation density tensor (ddt.) which is the central elastic invariant in Davini's theory. There has been some progress in describing the evolution of defects in the context of the geometrical theory, Epstein and Maugin [8], Epstein and Elżanowski [7], though it is based on geometrical ideas rather than on continuum mechanical balance laws.

To make some more detailed connection between the two theories, we ask the following question: "Is there a notion of material symmetry that is appropriate in Davini's theory?" In the geometrical theory, if w is the strain energy density of a uniform material, with respect to a uniform reference, the material symmetry group is the set of all linear transformations G such that

$$w(F) = w(FG), \quad \text{for all } F \in M_{3\times3}^+, \tag{1.1}$$

where $M_{3\times3}^+$ is the set of 3×3 matrices with positive determinant, and F represents a deformation gradient.

We   will   suppose that, in Davini's theory, there is defined an energy density function $\tilde{w} = \tilde{w}(\{\boldsymbol{\ell}_a\}, \mathcal{S})$, where $\boldsymbol{\ell}_1$, $\boldsymbol{\ell}_2$, $\boldsymbol{\ell}_3$ are three linearly independent vectors, $\{\boldsymbol{\ell}_a\}$ denotes the set $\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}$, and $\mathcal{S}$ is the ddt. Thus we adopt, as a constitutive hypothesis, the idea that point values of the frame and the ddt. are enough to determine the value of the energy at a point. Also, and this is a main assumption, we suppose that there is a crystal state $\Sigma \equiv \{\boldsymbol{\ell}_a(\cdot), \Omega; a = 1, 2, 3\}$, with corresponding ddt. uniform (i.e. constant in Ω), such that $\tilde{w}(\cdot)$ is also constant. So

$$\tilde{w}(\{\boldsymbol{\ell}_a(\boldsymbol{x})\}, \mathcal{S}) = \tilde{w}(\{\boldsymbol{\ell}_a(\boldsymbol{y})\}, \mathcal{S}), \quad \boldsymbol{x}, \boldsymbol{y} \in \Omega. \tag{1.2}$$

Defining the matrix field $L(\cdot)$ by

$$L(\boldsymbol{x})\boldsymbol{e}_a = \boldsymbol{\ell}_a(\boldsymbol{x}), \quad a = 1, 2, 3, \ x \in \Omega, \tag{1.3}$$

where e_1, e_2, e_3 is a canonical basis of $\mathbb{R}^3$, equation (1.2) may be put in the form

$$\tilde{w}(L(\boldsymbol{x}),\ \mathcal{S}) = \tilde{w}(L(\boldsymbol{y}),\ \mathcal{S}), \qquad (1.4)$$

with some rather slight abuse of notation. Phrased in this way, the state Σ is to define symmetry properties of $\tilde{w}(\cdot, \mathcal{S})$.

Reiterating, the assumption is that symmetries of the energy density define a frame with given constant ddt., if one accepts the smoothness of the frame and the connectedness of Ω. The issue that we shall investigate in this paper is the following – to what extent is this assumption compatible with the notion of symmetry that comes from equation (1.1) (which is isomorphic to the usual formulation of material symmetry in nonlinear elasticity theory)?

There   is   a superficial resemblance between (1.1) and (1.4); indeed if one takes $w(\cdot) = \tilde{w}(\cdot, \mathcal{S})$, $F = L(\boldsymbol{x})$, $G = (L(\boldsymbol{x}))^{-1}L(\boldsymbol{y})$, then there would seem to be a definite relationship if one could show that:

- there is an extension of $\tilde{w}(\cdot, \mathcal{S})$ from $L(\Omega)$ to all of $M_{3\times3}^+$ such that the 'analogue' of (1.4) holds (this is imprecisely stated, here),

- $\underset{\boldsymbol{y}\in\Omega}{\mathrm{range}}(L(\boldsymbol{x}))^{-1}L(\boldsymbol{y})$ is independent of $\boldsymbol{x}$.

The method that we shall use to investigate this issue (or rather, whether or not assumption (1.4) is viable) is based on the following:

(i) we focus on cases where ddt. is constant in Ω. This seems reasonable under the constitutive hypothesis that $\tilde{w}$ is independent of gradients of the ddt.. Then crystal state $\Sigma = \{L(\cdot), \Omega\}$ has a Lie group structure, Parry [13], so that there exists an (associative) Lie group composition function $\boldsymbol{\psi} : \Omega \times \Omega \to \Omega$ and the lattice vector fields $\boldsymbol{\ell}_1(\cdot)$, $\boldsymbol{\ell}_2(\cdot)$, $\boldsymbol{\ell}_3(\cdot)$, or $L(\cdot)$, have a self similarity property which corresponds to 'right invariance' with respect to the action of the group,

$$\boldsymbol{\ell}_a\left(\boldsymbol{\psi}\left(\boldsymbol{x}, \boldsymbol{y}\right)\right) = \nabla_1\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{\ell}_a(\boldsymbol{x}), \quad a = 1, 2, 3,\ \boldsymbol{x}, \boldsymbol{y} \in \Omega, \qquad (1.5)$$

where ∇_1 denotes the gradient with respect to the first argument. Note that (1.5) can also be written as

$$L\left(\boldsymbol{\psi}\left(\boldsymbol{x}, \boldsymbol{y}\right)\right) = \nabla_1\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y})L(\boldsymbol{x}), \quad \boldsymbol{x}, \boldsymbol{y} \in \Omega. \qquad (1.6)$$

(ii) The ddt. $\mathcal{S}$ is invariant under elastic deformation, and so elastic deformation of a crystal state with constant $\mathcal{S}$ produces a crystal state with constant $\mathcal{S}$.

(iii) It will turn out that, in all cases where $\mathcal{S}$ is singular, one can choose a crystal state (with the given, constant, $\mathcal{S}$) such that $\boldsymbol{\psi}$ is affine with respect to its first argument. We shall presume that (1.4) holds for the crystal state so defined, and then extend $\tilde{w}(\cdot, \mathcal{S})$ so that it is defined over $M_{3\times3}^+$ and some analogue of (1.4) holds. (In fact we partition $M_{3\times3}^+$ into disjoint sets such that equation (1.4) holds on each set.)

(iv) Choosing $\boldsymbol{\psi}$ as above ensures that the crystal states so constructed have a group property over and above the original Lie group structure. This group property is what allows a direct comparison with (1.1), and encourages us to say that the crystal states constructed in this way provide the material symmetry groups for $\tilde{w}(\cdot, \mathcal{S})$. These material symmetry groups depend on the ddt., in general.

The material symmetry groups that emerge are continuous groups. If one assumes that the function $\tilde{w}(\cdot, \mathcal{S})$ is also objective, then one can find representations of $\tilde{w}$ in terms of certain combinations of $L^T L$ ($L^T = L$ transposed), the analogue of the Green strain, in just the same way as one finds that the strain energy depends on the principal invariants of Green strain in classical nonlinear isotropic elasticity theory. But in this case the representation depends on the ddt., since that tensor determines the symmetry group. We find, for example, that for some choices of $\mathcal{S}$, the material can be regarded as transversely isotropic (with distinguished axis determined by $\mathcal{S}$), and we give examples of explicit representations of the strain energy function in some other cases where $\mathcal{S}$ is singular.

2.   Further motivation based on discrete structure

The symmetry groups of perfect discrete crystals are thoroughly investigated, by now. For a simple lattice K determined by a basis $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, $\boldsymbol{e}_3$,

$$K = \{\boldsymbol{x} : \boldsymbol{x} = n^a \boldsymbol{e}_a,\ n^a \text{ any integer}, \quad a = 1,\ 2,\ 3\}, \qquad (2.1)$$

one may study the space groups, the point groups, the lattice groups, and their various interrelationships. Similar problems of classification occur in the case of discrete defective crystals that arise from a continuous structure through an iteration process, see Parry[13], Cermelli and Parry [3], though these problems are neither classical nor thoroughly investigated (from the point of view of continuum mechanics). There,

a ddt. $\mathcal{S}$ is prescribed, and a frame with given $\mathcal{S}$ is constructed in some canonical fashion. A starting point $\boldsymbol{x}_0$ is chosen and a set of points is determined by flow along each of the three vector fields for time 1 (and time -1). The procedure is repeated with each of the set of six points so generated, and so on. In some cases the procedure determines a discrete set of points, and any such discrete set of points turns out to be a multilattice (i.e. a collection of congruent simple lattices). The symmetry properties of this multilattice may be investigated, Cermelli and Parry [3], Pitteri and Zanzotto [16]. The multilattice depends on $\boldsymbol{x}_0, \mathcal{S}$, and the starting values of the frame $\boldsymbol{\ell}_a(\boldsymbol{x}_0) \equiv \boldsymbol{\ell}_a$, $a = 1, 2, 3$, denote it $M(\boldsymbol{x}_0, \{\boldsymbol{\ell}_a\}, \mathcal{S})$.

Now the canonical procedure that is used to construct the frame, in cases that give multilattices, is the following; first follow a standard procedure, Pontryagin [17], to find a frame with given $\mathcal{S}$ and $\boldsymbol{\ell}_a(\mathbf{0}) = \boldsymbol{e}_a$. Then select an affine elastic deformation, with gradient F, that maps $\mathbf{0}$ to $\boldsymbol{x}_0$ and has $F\boldsymbol{e}_a = \boldsymbol{\ell}_a$. Since elastic deformation preserves the ddt., this particular elastic deformation produces a frame with 'starting point' $\boldsymbol{x}_0$, $\boldsymbol{\ell}_a(\boldsymbol{x}_0) = \boldsymbol{\ell}_a$ and ddt. $\mathcal{S}$, moreover the iteration procedure described above produces a multilattice $M(\boldsymbol{x}_0, \{\boldsymbol{\ell}_a\}, \mathcal{S})$.

The task is to describe symmetries of $M(\boldsymbol{x}_0, \{\boldsymbol{\ell}_a\}, \mathcal{S})$, constructed as above. First notice that Pontryagin's frame satisfies the right invariance condition (1.5), and that in cases we are interested in $\nabla_1 \psi(\boldsymbol{x}, \boldsymbol{y})$ is independent of $\boldsymbol{x}$ so that (1.5) represents an affine elastic deformation. That is, the frame is mapped to itself by elastic deformations of the form

$$\boldsymbol{x} \to \psi(\boldsymbol{x}, \boldsymbol{y}) \equiv \psi(\mathbf{0}, \boldsymbol{y}) + [\nabla_1 \psi(\mathbf{0}, \boldsymbol{y})] \boldsymbol{x}. \qquad (2.2)$$

Second it is a fact that the processes of iteration and elastic deformation commute. Therefore, in particular, the multilattice generated after elastic deformation of Pontryagin's frame is the elastic image of $M(\mathbf{0}, \{\boldsymbol{e}_a\}, \mathcal{S})$, and by definition this multilattice is

$$M(\psi(\mathbf{0}, \boldsymbol{y}), \ [\nabla_1 \psi(\mathbf{0}, \boldsymbol{y})] \boldsymbol{e}_a, \mathcal{S}) \equiv M(\bar{\boldsymbol{x}}_0, \{\bar{\boldsymbol{\ell}}_a\}, \mathcal{S})$$

if we put $\bar{\boldsymbol{x}}_0 \equiv \psi(\mathbf{0}, \boldsymbol{y})$, $\bar{\boldsymbol{\ell}}_a \equiv [\nabla_1 \psi(\mathbf{0}, \boldsymbol{y})] \boldsymbol{e}_a$.

Now choose

$$\bar{\boldsymbol{x}}_0 \equiv \psi(\mathbf{0}, \boldsymbol{y}) \in M(\mathbf{0}, \{\boldsymbol{e}_a\}, \mathcal{S}). \qquad (2.3)$$

Then the iteration process, after elastic deformation (2.2), with $\boldsymbol{y}$ given by (2.3), commences with a point of $M(\mathbf{0}, \{\boldsymbol{e}_a\}, \mathcal{S})$ and employs Pontryagin's frame by virtue of the right invariance condition. Therefore,

$$M(\mathbf{0}, \{\boldsymbol{e}_a\}, \mathcal{S}) = M(\bar{\boldsymbol{x}}_0, \{\bar{\boldsymbol{\ell}}_a\}, \mathcal{S}) = \bar{\boldsymbol{x}}_0 + [\nabla_1 \psi(\mathbf{0}, \boldsymbol{y})] M(\mathbf{0}, \{\boldsymbol{e}_a\}, \mathcal{S})$$

for all $\boldsymbol{y}$ such that (2.3) holds. But

$$M\left(\bar{\boldsymbol{x}}_0, \left\{\bar{\boldsymbol{\ell}}_a\right\}, \mathcal{S}\right) = \bar{\boldsymbol{x}}_0 + M\left(\boldsymbol{0}, \left\{\bar{\boldsymbol{\ell}}_a\right\}, \mathcal{S}\right)$$

according to the canonical procedure. So

$$M\left(\boldsymbol{0}, \left\{\boldsymbol{e}_a\right\}, \mathcal{S}\right) = M\left(\boldsymbol{0}, \left\{\boldsymbol{\ell}_a\right\}, \mathcal{S}\right)$$

whenever $\bar{\boldsymbol{\ell}}_a = [\nabla_1 \boldsymbol{\psi}\left(\boldsymbol{0}, \boldsymbol{y}\right)] \boldsymbol{e}_a$ and (2.3) holds.

Finally one imagines that the strain energy is determined by the relative positions of the points in the multilattice, not on their absolute positions relative to some coordinate system. So (2.2) suggests that we should adopt

$$\tilde{w}\left(\left\{\boldsymbol{e}_a\right\}, \mathcal{S}\right) = \tilde{w}\left(\left\{\tilde{\boldsymbol{\ell}}_a\right\}, \mathcal{S}\right) \tag{2.4}$$

as a symmetry of the strain energy function, provided that

$$\tilde{\boldsymbol{\ell}}_a = \boldsymbol{\ell}_a\left(\tilde{\boldsymbol{x}}_0\right), \quad \text{where} \quad \tilde{\boldsymbol{x}}_0 \in M\left(\boldsymbol{0}, \left\{\boldsymbol{e}_a\right\}, \mathcal{S}\right). \tag{2.5}$$

We take these remarks as a clear motivation for considering relations of the form (1.2) in the continuous case, for (2.4) is just the discrete version of that relation, where the domain of definition of the lattice vectors, Ω, is taken as $M\left(\boldsymbol{0}, \left\{\boldsymbol{e}_a\right\}, \mathcal{S}\right)$.

3. Preliminaries

In Davini's model, a crystal state Σ is defined by prescribing three linearly independent lattice vector fields $\boldsymbol{\ell}_1(\cdot)$, $\boldsymbol{\ell}_2(\cdot)$, $\boldsymbol{\ell}_3(\cdot)$ throughout a region Ω, so $\Sigma \equiv \{\boldsymbol{\ell}_a(\cdot), \Omega; \ a = 1, 2, 3\}$. We also choose to write

$$L(\boldsymbol{x})\boldsymbol{\ell}_a(\boldsymbol{0}) = \boldsymbol{\ell}_a(\boldsymbol{x}), \quad a = 1, 2, 3, \quad \boldsymbol{x} \in \Omega, \tag{3.1}$$

on occasion. Let $\boldsymbol{d}_1(\cdot)$, $\boldsymbol{d}_2(\cdot)$, $\boldsymbol{d}_3(\cdot)$ be the duals of the lattice vector fields, so

$$\boldsymbol{d}_a(\boldsymbol{x}) \cdot \boldsymbol{\ell}_b(\boldsymbol{x}) = \delta_{ab}, \quad \boldsymbol{d}_a(\boldsymbol{x}) \otimes \boldsymbol{\ell}_a(\boldsymbol{x}) = \text{id.}, \quad a, b, = 1, 2, 3, \ \boldsymbol{x} \in \Omega. \tag{3.2}$$

Also let $n(\cdot)$ be the determinant of the dual lattice vector fields,

$$n(\boldsymbol{x}) = \det\left\{\boldsymbol{d}_a(\boldsymbol{x})\right\} = \boldsymbol{d}_1(\boldsymbol{x}) \cdot \boldsymbol{d}_2(\boldsymbol{x}) \wedge \boldsymbol{d}_3(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{3.3}$$

and define $D(\cdot)$ by

$$D(\boldsymbol{x})\boldsymbol{d}_a(\boldsymbol{0}) = \boldsymbol{d}_a(\boldsymbol{x}), \quad a = 1, 2, 3, \ \boldsymbol{x} \in \Omega. \tag{3.4}$$

Then from (3.2),

$$D^T(\boldsymbol{x})L(\boldsymbol{x}) = \mathcal{I}, \quad \boldsymbol{x} \in \Omega \tag{3.5}$$

when T denotes the transposed matrix, and $\mathcal{I}$ is the 3×3 identity.

The dislocation density tensor (ddt.), at a given point $\boldsymbol{x} \in \Omega$, is the 3×3 matrix which has components

$$\mathcal{S}_{ab} = \nabla \wedge \boldsymbol{d}_a \cdot \boldsymbol{d}_b / n. \tag{3.6}$$

Note that

$$\nabla \wedge \boldsymbol{d}_a = n \, \mathcal{S}_{ab} \boldsymbol{\ell}_b, \tag{3.7}$$

by virtue of $(3.2)_2$, so that

$$0 = \nabla \cdot (\nabla \wedge \boldsymbol{d}_a) = \mathcal{S}_{ab} \nabla \cdot (n \boldsymbol{\ell}_b), \tag{3.8}$$

in the case that $\mathcal{S} \equiv (\mathcal{S}_{ab})$ is constant in Ω. This implies, Parry [13], that

$$\mathcal{S}_{ab} w_b = 0, \tag{3.9}$$

where (w_b) is the axial part of $\mathcal{S}$;

$$w_b \equiv \tfrac{1}{2} \epsilon_{brs} \mathcal{S}_{rs}. \tag{3.10}$$

In particular $\mathcal{S}$ is singular if it is not symmetric.

We remark at this point that, in the case that $\mathcal{S}$ is singular, the domain Ω can be taken as all of $\mathbb{R}^3$ (cf. Theorem 3).

An elastic deformation $\boldsymbol{y}$ of lattice vector fields $\boldsymbol{\ell}_a(\cdot)$, defined over Ω, produces lattice vector fields $\tilde{\boldsymbol{\ell}}_a(\cdot)$, defined over $\boldsymbol{y}(\Omega)$, given by

$$\tilde{\boldsymbol{\ell}}_a \left(\boldsymbol{y} \left(\boldsymbol{x} \right) \right) = \nabla \boldsymbol{y} \, \boldsymbol{\ell}_a(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega. \tag{3.11}$$

When (3.11) holds for some choice of the function $\boldsymbol{y} : \Omega \to \mathbb{R}^3$ one says that crystal states $\Sigma = \{\boldsymbol{\ell}_a(\cdot), \Omega; \ a = 1, 2, 3\}$, $\tilde{\Sigma} = \left\{ \tilde{\boldsymbol{\ell}}_a(\cdot), \boldsymbol{y}(\Omega); \ a = 1, 2, 3 \right\}$ are elastically related to one another.

Now we reiterate that the focus of this paper will be on crystal states when the ddt. is constant in Ω. The motivation for this is that the strain energy depends on $\{\boldsymbol{\ell}_a\}, \mathcal{S}$ alone – the idea is that the pair $\{\boldsymbol{\ell}_a\}$, $\mathcal{S}$ determines a 'local state' which, in the absence of any information about the gradients of the ddt., is thought to derive from fields $\boldsymbol{\ell}_a(\cdot)$ with constant ddt. equal to the given value $\mathcal{S}$, which take the values $\{\boldsymbol{\ell}_a\}$ at some relevant point $\boldsymbol{x}_0$, $\boldsymbol{\ell}_a(\boldsymbol{x}_0) = \boldsymbol{\ell}_a$, $1 = 1, 2, 3$.

Now the fact that $\mathcal{S}$ is constant implies that, given vector fields $\boldsymbol{\ell}_a(\cdot)$ with

$$\boldsymbol{\ell}_a(\boldsymbol{0}) = \boldsymbol{e}_a, \quad a = 1, 2, 3, \tag{3.12}$$

(with ddt. constant, satisfying (3.9), (3.10)), the differential system

$$\boldsymbol{\ell}_a \left(\boldsymbol{\psi} \left(\boldsymbol{x}, \boldsymbol{u} \right) \right) = \nabla_1 \boldsymbol{\psi} \left(\boldsymbol{x}, \boldsymbol{u} \right) \boldsymbol{\ell}_a(\boldsymbol{x}), \tag{3.13}$$

$$\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{0}) = \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{0}) = \boldsymbol{x}, \tag{3.14}$$

has a unique invertible solution $\boldsymbol{\psi} : \Omega \times \Omega \to \Omega$ such that

$$\boldsymbol{\psi}\left(\boldsymbol{u}, \boldsymbol{\psi}(\boldsymbol{v}, \boldsymbol{w})\right) = \boldsymbol{\psi}\left(\boldsymbol{\psi}(\boldsymbol{u}, \boldsymbol{v}), \boldsymbol{w}\right), \tag{3.15}$$

i.e. $\boldsymbol{\psi}$ is associative, and invertible in both arguments, Pontryagin [17]. Equation (3.13) expresses a self similarity property of vector fields $\boldsymbol{\ell}_a(\cdot)$ with constant ddt.; if one fixes the parameter $\boldsymbol{u}$ in (3.13) and puts $\boldsymbol{y}(\cdot) = \boldsymbol{\psi}(\cdot, \boldsymbol{u})$, (3.13) asserts that crystal state $\{\boldsymbol{\ell}_a(\cdot), \ \Omega\}$ is elastically related to crystal state $\{\boldsymbol{\ell}_a(\cdot), \ \boldsymbol{y}(\Omega)\}$, $\Omega \subseteq \mathbb{R}^3$. By allowing $\boldsymbol{u}$ to vary, and noting that $\boldsymbol{\psi}$ is invertible, one sees that the lattice vector fields in each neighbourhood of every point of Ω are elastically related to the (same) lattice vector fields in some neighbourhood of every other point in Ω.

Conditions (3.14) and (3.15) ensure that $\boldsymbol{\psi}$ defines a Lie group composition function with the origin $\boldsymbol{0}$ acting as the identity element of the group. In Lie group language, (3.13) expresses the right invariance of the lattice vector fields with respect to multiplication (of $\boldsymbol{x}$) by $\boldsymbol{u}$, on the right.

As a partial converse of this result (the existence of $\boldsymbol{\psi}$), note that if (3.13) holds, then the ddt. deriving from the fields $\boldsymbol{\ell}_a(\cdot)$ is necessarily constant; for any ddt. is an elastic invariant and (3.13) then implies

$$\mathcal{S}\left(\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u})\right) = \mathcal{S}(\boldsymbol{x}). \tag{3.16}$$

This implies that $\mathcal{S}$ is constant as $\boldsymbol{\psi}$ is invertible. The following lemma is a necessary slight generalization of the Pontryagin's result, replacing $\boldsymbol{0}$ by an arbitrary point $\boldsymbol{e}$, and relaxing condition (3.12).

LEMMA 1. *Suppose that fields $\boldsymbol{\ell}_a'(\cdot)$ are given, with $\mathcal{S}'$ constant and $\boldsymbol{\ell}_a'(\boldsymbol{e}) = \boldsymbol{\ell}_a'$, for some $\boldsymbol{e} \in \mathbb{R}^3$. Then there exists a unique associative group composition function $\boldsymbol{\psi}'$ such that*

$$\boldsymbol{\ell}_a'\left(\boldsymbol{\psi}'\left(\boldsymbol{x}', \boldsymbol{u}'\right)\right) = \nabla_1 \boldsymbol{\psi}'\left(\boldsymbol{x}', \boldsymbol{u}'\right) \boldsymbol{\ell}_a'(\boldsymbol{x}'), \tag{3.17}$$

$$\boldsymbol{\psi}'\left(\boldsymbol{x}', \boldsymbol{e}\right) = \boldsymbol{\psi}'\left(\boldsymbol{e}, \boldsymbol{x}'\right) = \boldsymbol{x}'. \tag{3.18}$$

PROOF

Define the matrix $\Gamma = (\gamma_{ab})$ uniquely by $\boldsymbol{\ell}_a' = \gamma_{ab} \boldsymbol{e}_b$. Define $\boldsymbol{\ell}_b(\cdot)$ by $\boldsymbol{\ell}_a'(\boldsymbol{x} + \boldsymbol{e}) = \gamma_{ab} \boldsymbol{\ell}_b(\boldsymbol{x})$. Then the fields $\boldsymbol{\ell}_a(\cdot)$ satisfy $\boldsymbol{\ell}_a(\boldsymbol{0}) = \boldsymbol{e}_a$, and one calculates that $\mathcal{S}' = (\det \Gamma) \Gamma^{-T} \mathcal{S} \Gamma^{-1}$, where $\mathcal{S}$ is the ddt. corresponding to the fields $\boldsymbol{\ell}_a(\cdot)$. Therefore according to Pontryagin's result, there exists a group composition function $\boldsymbol{\psi}$ satisfying (3.13), (3.14), (3.15) (for the fields $\boldsymbol{\ell}_b(\cdot)$ defined as above). Multiplying (3.13) by γ_{ab} gives

$$\boldsymbol{\ell}_a'\left(\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u}) + \boldsymbol{e}\right) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u}) \boldsymbol{\ell}_a'(\boldsymbol{x} + \boldsymbol{e}). \tag{3.19}$$

Put

$$\boldsymbol{\psi}'(\boldsymbol{x} + \boldsymbol{e},\ \boldsymbol{y} + \boldsymbol{e}) \equiv \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) + \boldsymbol{e}, \qquad (3.20)$$

to deduce that (3.17) holds for this choice of $\boldsymbol{\psi}'$, and use (3.14) and (3.15) to show that (3.18) and the analogue of (3.15) also hold.

Finally argue by contradiction (reversing the above argument) that this choice of $\boldsymbol{\psi}'$ is uniquely determined. ∎

REMARKS

- In Lemma 1, the point $\boldsymbol{e} \in \mathbb{R}^3$ acts as the group identity element, so far as multiplication defined by $\boldsymbol{\psi}'$ is concerned.

- The group composition function that appears in (3.17), (3.18) is unchanged if the fields $\boldsymbol{\ell}'_a(\cdot)$ are replaced by fields $\gamma'_{ab}\boldsymbol{\ell}'_b(\cdot)$, for any nonsingular $\Gamma' \equiv (\gamma'_{ab})$.

- Recall that the structure constants of the Lie algebra corresponding to the Lie group defined by $\boldsymbol{\psi}$ are C_{ijk}, $i, j, k = 1, 2, 3$, when $C_{ijk} = A_{ijk} - A_{ikj}$ and

$$A_{ijk} \equiv \frac{\partial^2 \psi_i}{\partial x_j \partial u_k}(\boldsymbol{0}, \boldsymbol{0}), \qquad (3.21)$$

(we refer to the case where $\boldsymbol{e} = \boldsymbol{0}$). So

$$C_{ijk} = \varepsilon_{sjk}\varepsilon_{spq}A_{ipq}. \qquad (3.22)$$

Also recall that if one calculates the Lie bracket, $\boldsymbol{L}_3(\cdot)$ say, of the pair of right invariant vector fields $\boldsymbol{\ell}_1(\cdot)$ and $\boldsymbol{\ell}_2(\cdot)$, then $\boldsymbol{L}_3(\cdot)$ is itself right invariant, with the same composition function. Moreover,

$$\boldsymbol{L}_3(\boldsymbol{0}) = [(\boldsymbol{\ell}_1 \cdot \nabla)\,\boldsymbol{\ell}_2 - (\boldsymbol{\ell}_2 \cdot \nabla)\,\boldsymbol{\ell}_1]\,(\boldsymbol{0}) \qquad (3.23)$$

and a calculation shows that

$$L_{3i}(\boldsymbol{0}) = C_{ijk}\ell_{1j}(\boldsymbol{0})\ell_{2k}(\boldsymbol{0}), \qquad (3.24)$$

where C_{ijk} is given by (3.22). Clearly one may write

$$L_3(\boldsymbol{0}) = \tilde{C}_{k12}\boldsymbol{\ell}_k(\boldsymbol{0}), \qquad (3.25)$$

for some constants $\tilde{C}_{k12}$. From (3.24) and (3.25)

$$\tilde{C}_{k12}\ell_{ki}(\boldsymbol{0}) = C_{ijk}\ell_{1j}(\boldsymbol{0})\ell_{2k}(\boldsymbol{0}), \qquad (3.26)$$

and in general, choosing $\tilde{C}_{krs}$ antisymmetric,

$$\tilde{C}_{krs}\ell_{ki}(\boldsymbol{0}) = C_{ijk}\ell_{rj}(\boldsymbol{0})\ell_{sk}(\boldsymbol{0}). \qquad (3.27)$$

One may abstract these calculations by noting that the Lie bracket provides   an antisymmetric bilinear operation from pairs of right invariant fields, to the vector space of right invariant fields. The right invariant fields are determined by their values at the origin, so one may introduce an antisymmetric bilinear mapping of $\mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3$ by

$$[\boldsymbol{\ell}_r, \boldsymbol{\ell}_s] = \tilde{C}_{krs} \boldsymbol{\ell}_r, \tag{3.28}$$

and the study of Lie algebras starts with (3.28).

Note that, if the composition function is given, then the values of the constants $\tilde{C}_{krs}$ depend on initial values of the right invariant fields chosen to act as a basis for the vector space of all such fields, from (3.27).

– Take the scalar product of (3.25) with $\boldsymbol{d}_\ell(0)$ to get

$$\boldsymbol{L}_3(0) \cdot \boldsymbol{d}_\ell(0) = \tilde{C}_{\ell 12}, \tag{3.29}$$

so that

$$\boldsymbol{L}_k(0) \cdot \boldsymbol{d}_\ell(0) = \tfrac{1}{2} \varepsilon_{krs} \tilde{C}_{\ell rs}, \tag{3.30}$$

in general. But from Parry and Šilhavý [14],

$$\boldsymbol{L}_k \cdot \boldsymbol{d}_\ell = \mathcal{S}_{\ell k}, \tag{3.31}$$

so

$$\mathcal{S}_{\ell k} = \tfrac{1}{2} \varepsilon_{krs} \tilde{C}_{\ell rs}, \quad \tilde{C}_{\ell pq} = \varepsilon_{kpq} \mathcal{S}_{\ell k}. \tag{3.32}$$

Thus, equation (3.27) and (3.32) together provide a relation between the ddt., the composition function, and the initial values of the right invariant fields chosen to calculate the ddt..

– If $\mathcal{S}$ is the ddt. calculated from a given composition function, and fields $\boldsymbol{\ell}_a(\cdot)$ are such that $\boldsymbol{\ell}_a(\boldsymbol{0}) = \boldsymbol{e}_a$, $a = 1, 2, 3$, then it is clear from the definition of ddt. that if the fields $\boldsymbol{\ell}_a(\cdot)$ are replaced by fields $\boldsymbol{\ell}_a^*(\cdot) = \gamma_{ab} \boldsymbol{\ell}_a(\cdot)$, then the ddt. is changed to $\mathcal{S}^*$ defined by

$$\mathcal{S}^* = (\det \Gamma) \Gamma^{-T} \mathcal{S} \Gamma^{-1} \tag{3.33}$$

where the matrix Γ has components (γ_{ab}). This relation is easily reconciled with (3.27) and (3.32).

4. Sufficient condition

Here we introduce sufficient conditions, related to the assumption that

$$\tilde{w}\left(\{\boldsymbol{\ell}_a(\boldsymbol{x})\},\mathcal{S}\right) = \tilde{w}\left(\{\boldsymbol{\ell}_a(\boldsymbol{y}),\},\mathcal{S}\right), \quad \boldsymbol{x},\boldsymbol{y},\in \Omega, \tag{4.1}$$

which guarantee that one can then introduce a 'material symmetry' group in a fashion analogous to the continuum mechanics of simple materials.

First write (4.1) as

$$\tilde{w}\left(L(\boldsymbol{x}),\mathcal{S}\right) = \tilde{w}\left(L(\boldsymbol{\psi}),\mathcal{S}\right), \tag{4.2}$$

recalling (1.3) and putting $\boldsymbol{y} \equiv \boldsymbol{\psi} \equiv \boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u})$. Then formally (thinking of $L(\boldsymbol{\psi})$), say, as a matrix irrespective of the point of application)

$$\tilde{w}\left(L(\boldsymbol{x}),\mathcal{S}\right) = \tilde{w}\left(L(\boldsymbol{x})\left(L(\boldsymbol{x})^{-1}L(\boldsymbol{\psi})\right),\mathcal{S}\right). \tag{4.3}$$

But from right invariance (1.6)

$$L(\boldsymbol{x})^{-1}L(\boldsymbol{\psi}) = L(\boldsymbol{x})^{-1}\left[\nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u})\right]L(\boldsymbol{x}), \tag{4.4}$$

and we are interested in the question of whether or not, for fixed $\boldsymbol{x}$, the set of matrices defined by

$$F_{\boldsymbol{x}} = \left\{H : H = \nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u}),\ \boldsymbol{u} \in \mathbb{R}^3\right\}, \tag{4.5}$$

is a group. For if $F_{\boldsymbol{x}}$ is a group, so is $L(\boldsymbol{x})^{-1}F_{\boldsymbol{x}}L(\boldsymbol{x})$. (Note that in (4.5), Ω is taken equal to $\mathbb{R}^3$, a fact that will be justified in Theorem 3 in the case that $\mathcal{S}$ is singular).

THEOREM 2. *Let $F_{\boldsymbol{x}}$ be defined by (4.5). Then (i) $F_{\boldsymbol{x}} = F_{\boldsymbol{y}}$ if $L(\boldsymbol{x}) = L(\boldsymbol{y})$, and (ii) if $F_{\boldsymbol{x}}$ is independent of $\boldsymbol{x}$, then $F_{\boldsymbol{x}}$ is a group.*

PROOF

(i) Let $\boldsymbol{y} = \boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u})$, $L(\boldsymbol{x}) = L(\boldsymbol{y})$. Then $\nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y}) = \mathcal{I}$ from (1.6). By differentiating (3.15) with respect to the first argument one obtains:

$$\nabla_1\boldsymbol{\psi}\left(\boldsymbol{\psi}(\boldsymbol{v},\boldsymbol{w}),\boldsymbol{z}\right)\nabla_1\boldsymbol{\psi}(\boldsymbol{v},\boldsymbol{w}) = \nabla_1\boldsymbol{\psi}(\boldsymbol{v},\boldsymbol{\psi}(\boldsymbol{w},\boldsymbol{z})). \tag{4.6}$$

Putting $\boldsymbol{v} = \boldsymbol{x},\boldsymbol{w} = \boldsymbol{u},\nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u}) = \mathcal{I}$, this becomes

$$\nabla_1\boldsymbol{\psi}\left(\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u}),\boldsymbol{w}\right) = \nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{\psi}(\boldsymbol{u},\boldsymbol{w})), \tag{4.7}$$

that is

$$\nabla_1\boldsymbol{\psi}\left(\boldsymbol{y},\boldsymbol{w}\right) = \nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{\psi}(\boldsymbol{u},\boldsymbol{w})), \tag{4.8}$$

where $\boldsymbol{y} = \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u})$ determines $\boldsymbol{u}$ in terms of $\boldsymbol{x}$ and $\boldsymbol{y}$. It is convenient to use a different notation for the group multiplication of two elements $\boldsymbol{a}, \boldsymbol{b}$: put $\boldsymbol{\psi}(\boldsymbol{a}, \boldsymbol{b}) = \boldsymbol{a} \cdot \boldsymbol{b}$, and also let $\boldsymbol{a}^{-1}$ be such that $\boldsymbol{\psi}(\boldsymbol{a}, \boldsymbol{a}^{-1}) = \boldsymbol{\psi}(\boldsymbol{a}^{-1}, \boldsymbol{a}) = \boldsymbol{0}$. Then returning to (4.8), $\boldsymbol{y} = \boldsymbol{x} \cdot \boldsymbol{u}$, so $\boldsymbol{u} = \boldsymbol{x}^{-1} \cdot \boldsymbol{y}$ and (4.8) reads

$$\nabla_1 \boldsymbol{\psi} \left(\boldsymbol{y}, \boldsymbol{w} \right) = \nabla_1 \boldsymbol{\psi} \left(\boldsymbol{x}, (\boldsymbol{x}^{-1} \cdot \boldsymbol{y}) \cdot \boldsymbol{w} \right). \tag{4.9}$$

Now it is clear that $(\boldsymbol{x}^{-1} \cdot \boldsymbol{y}) \cdot \boldsymbol{w}$ ranges over the group $(\mathbb{R}^3)$ as $\boldsymbol{w}$ takes all values in the group, and vice versa. This proves that $F_{\boldsymbol{x}} = F_{\boldsymbol{y}}$.

(ii) Suppose that $F_{\boldsymbol{x}} = F_{\boldsymbol{0}}$ for all $\boldsymbol{x} \in \mathbb{R}^3$. Then

$$\nabla_1 \boldsymbol{\psi} \left(\boldsymbol{x}, \boldsymbol{u} \right) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{p}(\boldsymbol{x}, \boldsymbol{u})), \tag{4.10}$$

for some invertible $p(\boldsymbol{x}, \cdot)$.

To show that $F_{\boldsymbol{0}}$ is a group, it is sufficient to demonstrate that

$$\nabla_1 \boldsymbol{\psi} \left(\boldsymbol{0}, \boldsymbol{x} \right) \left[\nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{y}) \right]^{-1} = \nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{z}), \tag{4.11}$$

for some $\boldsymbol{z} = \boldsymbol{z}(\boldsymbol{x}, \boldsymbol{y})$. Putting $\boldsymbol{v} = \boldsymbol{0}$ in (4.7),

$$\nabla_1 \boldsymbol{\psi}(\boldsymbol{w}, \boldsymbol{z}) \nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{w}) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{\psi}(\boldsymbol{w}, \boldsymbol{z})). \tag{4.12}$$

Therefore, with $\boldsymbol{v}$ and $\boldsymbol{\psi}(\boldsymbol{w}, \boldsymbol{z}) = \boldsymbol{q}$ fixed,

$$\begin{aligned}
\nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{q}) \left[\nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{w}) \right]^{-1} &= \nabla_1 \boldsymbol{\psi}(\boldsymbol{w}, \boldsymbol{z}) \\
&= \nabla_1 \boldsymbol{\psi}(\boldsymbol{w}, \boldsymbol{w}^{-1} \cdot q) \\
&= \nabla_1 \boldsymbol{\psi} \left(\boldsymbol{0}, \boldsymbol{p}(\boldsymbol{w}, \boldsymbol{w}^{-1} \cdot \boldsymbol{q}) \right),
\end{aligned} \tag{4.13}$$

using the alternative notation for group multiplication, and (4.10). This proves (4.11) by appropriate renaming of variables. ∎

In the sequel, we shall investigate a more stringent condition than $F_{\boldsymbol{x}} = F_{\boldsymbol{0}}$, $\boldsymbol{x} \in \mathbb{R}^3$. We shall construct, in the case that $\mathcal{S}$ is singular, composition functions $\boldsymbol{\psi}$ such that, for each $\boldsymbol{u} \in \mathbb{R}^3$,

$$\nabla_1 \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u}) = \nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{u}), \quad \boldsymbol{x} \in \mathbb{R}^3. \tag{4.14}$$

Since $\nabla_1 \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u})$ is to be independent of $\boldsymbol{x}$, it follows that $\boldsymbol{\psi}$ is affine in its first argument,

$$\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u}) = \boldsymbol{u} + g(\boldsymbol{u})\boldsymbol{x} \tag{4.15}$$

for some function $g(\cdot)$ such that $g(\boldsymbol{0}) = \mathcal{I}$, using $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{0}) = \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{x}) = \boldsymbol{x}$. Since $\boldsymbol{\psi}$ is to be associative, it follows that $\boldsymbol{g}(\cdot)$ must be such that

$$[\boldsymbol{w} + g(\boldsymbol{w})\boldsymbol{v}] + g(\boldsymbol{\psi}(\boldsymbol{v}, \boldsymbol{w}))\boldsymbol{u} = \boldsymbol{w} + g(\boldsymbol{w}) [\boldsymbol{v} + g(\boldsymbol{v})\boldsymbol{u}]. \tag{4.16}$$

Thus

$$g\left(\boldsymbol{\psi}(\boldsymbol{v},\boldsymbol{w})\right) = g(\boldsymbol{w})g(\boldsymbol{v}). \qquad (4.17)$$

(It follows that $g^{T}(\cdot)$ provides a matrix representation of the relevant Lie group). When (4.17) holds, the right invariance condition (3.13) becomes

$$\boldsymbol{\ell}_a(\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u})) = g(\boldsymbol{u})\boldsymbol{\ell}_a(\boldsymbol{x}). \qquad (4.18)$$

Note that, if $\boldsymbol{u}$ is regarded as fixed, this condition represents a *homogeneous* elastic deformation of crystal state $\Sigma = \{\boldsymbol{\ell}_a(\cdot), \Omega\}$. Note also that (4.18) and (1.3) imply that

$$L\left(\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u})\right) = g(\boldsymbol{u})L(\boldsymbol{x}) \qquad (4.19)$$

where $L(\boldsymbol{0}) = \mathcal{I}$ if $\boldsymbol{\ell}_a(\boldsymbol{0}) = \boldsymbol{e}_a$, $a = 1, 2, 3$. So, in particular, in the case that $\boldsymbol{\ell}_a(\boldsymbol{0}) = \boldsymbol{e}_a$,

$$L(\boldsymbol{u}) = g(\boldsymbol{u}). \qquad (4.20)$$

Then (4.17) can be written as

$$L\left(\boldsymbol{\psi}(\boldsymbol{v},\boldsymbol{w})\right) = L(\boldsymbol{w})L(\boldsymbol{v}), \qquad (4.21)$$

which one may regard as a 'multiplication law' for the lattice vector fields, in the case that $\boldsymbol{\psi}$ is affine is its first argument.

5. Elastic deformation, change of basis

We have seen in the previous section that, in order that certain crystal states with constant ddt. have a particular group structure, so far as (4.1) is concerned, it is sufficient that the corresponding composition function be affine in its first argument. Now let $\boldsymbol{\psi}$ be the composition function for a crystal state $\Sigma \equiv \{\boldsymbol{\ell}_a(\cdot), \Omega\}$ with constant ddt. $\mathcal{S}$. Let $\tilde{\Sigma} \equiv \left\{\tilde{\boldsymbol{\ell}}_a(\cdot), \boldsymbol{y}(\Omega)\right\}$ be elastically related to Σ, with deformation $\boldsymbol{y} : \Omega \to \mathbb{R}^3$. Then the composition function for $\tilde{\boldsymbol{\Sigma}}$ is defined by

$$\tilde{\boldsymbol{\psi}}\left(\boldsymbol{y}(\boldsymbol{x}), \boldsymbol{y}(\boldsymbol{u})\right) = \boldsymbol{y}\left(\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{u})\right), \quad \boldsymbol{x}, \boldsymbol{u} \in \Omega \qquad (5.22)$$

Moreover the state $\tilde{\Sigma}$ has the same constant ddt. $\mathcal{S}$. The flexibility afforded by equation (5.22) will enable us to find a $\tilde{\boldsymbol{\psi}}$ affine in its first argument in the case that $\mathcal{S}$ is singular.

In fact we shall be more specific than this – our goal is to discuss symmetries of the energy function $\tilde{w}\left(\{\boldsymbol{\ell}_a(\boldsymbol{x})\}, \mathcal{S}\right)$. So we shall construct states $\Sigma = \{\boldsymbol{\ell}_a(\cdot), \Omega\}$ which have the properties, given *values* $\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3 \in \mathbb{R}^3$, given $\mathcal{S}$ satisfying the (analogue of the) Jacobi identity, and given $\boldsymbol{e} \in \Omega$;

1) $\boldsymbol{\ell}_a(\boldsymbol{e}) = \boldsymbol{\ell}_a, \quad a = 1, 2, 3,$

2) $\mathcal{S}$ is the ddt. for state Σ,

3) the corresponding $\boldsymbol{\psi}$ is affine in its first argument.

The crystal state so constructed will provide a group of symmetry transformations $F_{\boldsymbol{e}}$, independent of the choice of the point $\boldsymbol{e}$ by virtue of property 3). That is, one has that

$$\tilde{w}\left(L(\boldsymbol{x}), \mathcal{S}\right) = \tilde{w}\left(L(\boldsymbol{x})\left(L(\boldsymbol{x})^{-1}FL(\boldsymbol{x})\right), \mathcal{S}\right), \ F \in F_{\boldsymbol{e}}. \qquad (5.23)$$

Notice that the pair $\{\boldsymbol{\ell}_a, \mathcal{S}\}$ determines a corresponding Lie algebra structure. It will be productive to consider the classification of three dimensional Lie algebras. Recall that if fields $\boldsymbol{\ell}_a(\cdot)$ are replaced by fields $\gamma_{ab}\boldsymbol{\ell}_b(\cdot)$, then the composition function is unchanged, but that the ddt. is changed according to (3.21). By using the equivalence between ddt. $\mathcal{S}$ and constants $\tilde{C}_{\ell rs}$ exhibited in (3.32), one sees that (3.33)(or (3.27)) is equivalent to

$$\tilde{C}_{krs}\gamma_{ki} = C_{ijk}\gamma_{rj}\gamma_{sk}, \qquad (5.24)$$

where $\tilde{C}_{krs}$ are calculated for state $\{\gamma_{ab}\boldsymbol{\ell}_b(\cdot), \Omega\}$ according to (3.25), and C_{ijk} is calculated directly from the composition function, according to (3.21), (3.22). Each state $\{\gamma_{ab}\boldsymbol{\ell}_b(\cdot), \Omega\}$, $\gamma = (\gamma_{ab})$ non-singular, has the same composition function as state $\{\boldsymbol{\ell}_a(\cdot), \Omega\}$.

Equation (5.24) defines an equivalence relation on constants $\tilde{C}_{krs}$ satisfying the Jacobi identity. The space of those constants is thereby partitioned into disjoint equivalence classes, elements of any one equivalence class sharing a single composition function. So if one can show that, for a particular choice of right invariant fields in a particular equivalence class, that the corresponding $\boldsymbol{\psi}$ is affine in its first argument, then one can find a choice of right invariant fields for which $\boldsymbol{\psi}$ is affine in its first argument for each $\tilde{C}_{krs}$ in that equivalence class.

Regarding C_{krs} as the structure constants of a Lie algebra, so $[\boldsymbol{\ell}_r, \boldsymbol{\ell}_s] = C_{krs}\boldsymbol{\ell}_k$ from (3.28), and replacing $\boldsymbol{\ell}_r$ by $\tilde{\boldsymbol{\ell}}_r = \gamma_{rs}\boldsymbol{\ell}_s$, one sees that $\left[\tilde{\boldsymbol{\ell}}_r, \tilde{\boldsymbol{\ell}}_s\right] = \tilde{C}_{krs}\tilde{\boldsymbol{\ell}}_k$ where $\tilde{C}_{krs}$ satisfies (5.24). Finding the disjoint equivalence classes of (5.24) therefore amounts to classifying the three dimensional Lie algebras with respect to the equivalence induced by a change of basis. One may turn to Jacobson [11] for the relevant classification (see also Belinfante [1], Capriz and Davini [2]).

So, following Jacobson [11] for the most part, we list the bracket relationships (3.28), and the non zero components of C_{krs} to within the antisymmetry $C_{krs} = -C_{ksr}$, for some element of each equivalence class defined by the relationship (5.24);

(i) $[\boldsymbol{\ell}_1, \boldsymbol{\ell}_2] = [\boldsymbol{\ell}_2, \boldsymbol{\ell}_3] = [\boldsymbol{\ell}_3, \boldsymbol{\ell}_1] = \mathbf{0}$,

(ii) $[\boldsymbol{\ell}_1, \boldsymbol{\ell}_2] = \boldsymbol{\ell}_3$, $[\boldsymbol{\ell}_2, \boldsymbol{\ell}_3] = [\boldsymbol{\ell}_3, \boldsymbol{\ell}_1] = \mathbf{0}$; $C_{312} = 1$,

(iii) $[\boldsymbol{\ell}_1, \boldsymbol{\ell}_2] = \boldsymbol{\ell}_1$, $[\boldsymbol{\ell}_1, \boldsymbol{\ell}_3] = [\boldsymbol{\ell}_2, \boldsymbol{\ell}_3] = \mathbf{0}$; $C_{112} = 1$,

(iv) Jacobson shows that, for this equivalence class, there is a choice of basis such that

$$[\boldsymbol{\ell}_1, \boldsymbol{\ell}_2] = \mathbf{0}, \ [\boldsymbol{\ell}_1, \boldsymbol{\ell}_3] = \alpha \boldsymbol{\ell}_1 + \beta \boldsymbol{\ell}_2, \ [\boldsymbol{\ell}_2, \boldsymbol{\ell}_3] = \gamma \boldsymbol{\ell}_1 + \delta \boldsymbol{\ell}_2,$$

where $A = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ is a non-singular matrix. He then notes that there is a further change of basis such that A is replaced by $\rho M^{-1} A M$, where $\rho \in \mathbb{R}$ is non zero, and M is a non singular 2×2 matrix. Then he assumes that the relevant field is algebraically closed, which we cannot do. But in our case A may be put into rational canonical form by similarity transformation. So, A has either zero or two real eigenvalues, in the first case $\{\boldsymbol{\nu}, A\boldsymbol{\nu}\}$ is a basis of $\mathbb{R}^2$ for any $\boldsymbol{\nu} \in \mathbb{R}^2$ and the action of A on this basis is $\boldsymbol{\nu} \to A\boldsymbol{\nu}$, $A\boldsymbol{\nu} \to A^2\boldsymbol{\nu} = -a\boldsymbol{\nu} + b\, A\boldsymbol{\nu}$, where $a = \det A$, $b = tr\, A$ and $b^2 < 4a$. Hence A may be represented as $\begin{pmatrix} 0 & -a \\ 1 & b \end{pmatrix}$, with no further simplification possible by choosing ρ appropriately. In the second case there is at least one real eigenvector, call it $\boldsymbol{\nu}$, and let $\boldsymbol{\nu}, \boldsymbol{\theta}$ be linearly independent. Then $A\boldsymbol{\nu} = k\boldsymbol{\nu}$, $A\boldsymbol{\theta} = \ell\boldsymbol{\nu} + m\boldsymbol{\theta}$, for some $k, \ell, m \in \mathbb{R}$, and A may be represented as $\begin{pmatrix} k & \ell \\ 0 & m \end{pmatrix}$, with $km \neq 0$. Letting $\rho = (km)^{1/2}$, A can be further simplified to $\begin{pmatrix} \pi & \ell \\ 0 & \pi^{-1} \end{pmatrix}$, (where $\pi = (k/m)^{1/2}$). Therefore one has that, in this case, either

$$[\boldsymbol{\ell}_1, \boldsymbol{\ell}_2] = \mathbf{0}, \ [\boldsymbol{\ell}_1, \boldsymbol{\ell}_3] = -a\boldsymbol{\ell}_2, \ [\boldsymbol{\ell}_2, \boldsymbol{\ell}_3] = \boldsymbol{\ell}_1 + b\boldsymbol{\ell}_2; \quad C_{213} = -a, \ C_{123} = 1, \ C_{223} = b,$$

or

$$[\boldsymbol{\ell}_1, \boldsymbol{\ell}_2] = \mathbf{0}, \ [\boldsymbol{\ell}_1, \boldsymbol{\ell}_3] = \pi\boldsymbol{\ell}_1 + \ell\boldsymbol{\ell}_2, \ [\boldsymbol{\ell}_2, \boldsymbol{\ell}_3] = \pi^{-1}\boldsymbol{\ell}_2; \quad C_{113} = \pi, \ C_{213} = \ell, \ C_{223} = \pi^{-1}.$$

(v) $[\boldsymbol{\ell}_1, \boldsymbol{\ell}_2] = \boldsymbol{\ell}_3$, $[\boldsymbol{\ell}_2, \boldsymbol{\ell}_3] = \pm\boldsymbol{\ell}_1$, $[\boldsymbol{\ell}_3, \boldsymbol{\ell}_1] = \boldsymbol{\ell}_2$; $C_{312} = 1$, $C_{123} = \pm 1$, $C_{231} = 1$.

Finally, by using the relationship between the structure constants and the ddt., one has the corresponding non zero values of $(\mathcal{S}_{ab})$ for an element of each equivalence class;

(i) all elements zero,

(ii) $\mathcal{S}_{33} = 1$,

(iii) $\mathcal{S}_{13} = 1$,

(iv) $\mathcal{S}_{22} = a$, $\mathcal{S}_{11} = 1$, $\mathcal{S}_{21} = b$, when $b^2 < 4a$, or $\mathcal{S}_{12} = \pi^{-1}$, $\mathcal{S}_{22} = \ell$, $\mathcal{S}_{21} = \pi^{-1}$,

(v) $\mathcal{S}_{33} = 1$, $\mathcal{S}_{11} = \pm 1$, $\mathcal{S}_{22} = 1$.

6. Affine composition function

Now we confine attention to cases where $\mathcal{S}$ is singular, and so dismiss case (v) above from the considerations below. (The work in this paper should be relevant for the treatment of the mechanics of neutral deformations, where $\mathcal{S}$ is singular, in particular for the case where $\mathcal{S}$ is constant.) The case where $\mathcal{S}$ is not singular is not considered.

Then, using the results from the previous section, by suitable relabelling one can assume that $\mathcal{S}$ has the form

$$\mathcal{S} = \begin{pmatrix} * & * & 0 \\ & * & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{6.1}$$

when the symbol $*$ denotes a possibly non-zero element. This is all the information we shall need from the previous section.

It will be relevant later on that if $\mathcal{S}$ is a 3×3 matrix with the block structure (6.1), the matrix $e^{\mathcal{S}}$ defined by

$$e^{\mathcal{S}} = \sum_{j \geq 0} \mathcal{S}^j / j!, \tag{6.2}$$

has the block structure

$$e^{\mathcal{S}} = \begin{pmatrix} * & * & 0 \\ & * & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{6.3}$$

We were led to the following theorem by brute force computation of the composition function in cases where $\mathcal{S}$ is singular, e.g. if $\mathcal{S} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}$, $\alpha > 0$, one can choose $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{y} + R(\boldsymbol{y})\boldsymbol{x}$, where

$$R(\boldsymbol{y}) = \begin{pmatrix} \cosh \sqrt{\alpha} y_3 & -\frac{1}{\sqrt{\alpha}} \sinh \sqrt{\alpha} y_3 & 0 \\ -\sqrt{\alpha} \sinh \sqrt{\alpha} y_3 & \cosh \sqrt{\alpha} y_3 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{6.4}$$

and the addition formulas for $\cosh(\cdot)$ and $\sinh(\cdot)$ give the required multiplication law for $R(\cdot)$.

There is probably a deeper reason why the following result should be true (the proof does not provide it).

THEOREM 3. *Let (singular) $\mathcal{S}$ have the form (6.1), then one can choose*

$$\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y}) = \boldsymbol{y} + e^{-y_3 C}\boldsymbol{x}, \qquad (6.5)$$

where C has components $C_{ir} \equiv \varepsilon_{ra3}\mathcal{S}_{ia}$.

PROOF

One has to verify that $\boldsymbol{\psi}$ is a composition function, and one has to check that the ddt. of corresponding right invariant fields is constant.

(a) First note that the third component of $\boldsymbol{\psi}(\boldsymbol{v},\boldsymbol{w})$ is $v_3 + w_3$, as $e^{-w_3 C}$ has the form (6.3). Then

$$\begin{aligned}
\boldsymbol{\psi}\left(\boldsymbol{\psi}\left(\boldsymbol{u},\boldsymbol{v}\right),\boldsymbol{w}\right) &= \boldsymbol{w} + e^{-w_3 C}\left(\boldsymbol{v} + e^{-v_3 C}\right) \\
&= \left(\boldsymbol{w} + e^{-w_3 C}\boldsymbol{v}\right) + e^{-(w_3+v_3)C}\boldsymbol{u} = \boldsymbol{\psi}\left(\boldsymbol{u},\boldsymbol{\psi}(\boldsymbol{v},\boldsymbol{w})\right).
\end{aligned} \qquad (6.6)$$

Also $\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{0}) = \boldsymbol{\psi}(\boldsymbol{0},\boldsymbol{x}) = \boldsymbol{x}$.

(b) From (6.5), $L(\boldsymbol{x}) = e^{-x_3 C}$, so $D(x) = e^{x_3 C^T}$. Therefore

$$\boldsymbol{d}_a(\boldsymbol{x}) = e^{x_3 C^T}\boldsymbol{e}_a, \quad d_{ai} = \left(e^{x_3 C}\right)_{ai}, \qquad (6.7)$$

and if one writes D in components as (D_{ai}) then $D_{ai} = d_{ia}$. Now, denoting differentiation with respect to x_3 as a superposed dot,

$$\dot{D} = C^T D = D C^T \qquad (6.8)$$

as C^T and $e^{x_3 C^T}$ commute. Therefore

$$\dot{d}_{ia} \equiv d_{ia,3} = C_{ip}d_{pa} = d_{ip}C_{pa}. \qquad (6.9)$$

Using these facts one calculates

$$(\nabla \wedge \boldsymbol{d}_a)_k = \varepsilon_{krs}d_{as,r} = \varepsilon_{k3s}\dot{d}_{as} = \varepsilon_{k3s}C_{ap}d_{ps}, \qquad (6.10)$$

so that

$$\begin{aligned}
\nabla \wedge \boldsymbol{d}_a \cdot \boldsymbol{d}_b &= \varepsilon_{k3s}d_{ps}d_{bk}C_{ap} = \varepsilon_{k\ell s}d_{bk}\delta_{3\ell}d_{ps}C_{ap} \\
&= \varepsilon_{k\ell s}d_{bk}d_{3\ell}d_{ps}C_{ap} = \varepsilon_{b3p}nC_{ap}
\end{aligned} \qquad (6.11)$$

Therefore C must be such that

$$\mathcal{S}_{ab} = \varepsilon_{b3p}C_{ap}. \qquad (6.12)$$

Clearly the components C_{a3} do not enter into relation (6.12), so we may impose that $C_{a3} = 0$. Then multiplying (6.12) by ε_{b3k} gives

$$\varepsilon_{b3k}\mathcal{S}_{ab} = (\delta_{33}\delta_{kp} - \delta_{3p}\delta_{k3})\,C_{ap} \;=\; \begin{aligned} &C_{ak} - \delta_{k3}C_{a3} \\ &= C_{ak}, \end{aligned} \tag{6.13}$$

as stated.   ∎

REMARKS

— Equation (6.5) defines $\boldsymbol{\psi}$ over $\mathbb{R}^3\times\mathbb{R}^3$ from which one may generate corresponding fields $\boldsymbol{\ell}_a(\cdot)$ over $\mathbb{R}^3$. This shows that, when $\mathcal{S}$ is singular, the fields $\boldsymbol{\ell}_a(\cdot)$ may be defined over $\mathbb{R}^3$.

— The theorem implies that, independently of any constitutive assumptions, crystal states deriving from right invariant fields corresponding to composition function (6.5) have a particular group structure. Indeed, the set of linear transformations that map a frame at any given point to all other frames in the crystal state is a group. Also, as proved earlier, this group is independent of the point that is selected initially.

7. Material symmetry

In this section we attempt to relate assumption (4.1) to the 'usual' definition of material symmetry in continuum mechanics. We are investigating the assumption that

$$\tilde{w}(L(\boldsymbol{\psi}), \mathcal{S}) = \tilde{w}(L(\boldsymbol{x}), \mathcal{S}), \tag{7.1}$$

and have noted already that

$$L(\boldsymbol{\psi})L(\boldsymbol{x})^{-1} = \nabla_1\boldsymbol{\psi}(\boldsymbol{x},\ \boldsymbol{y}). \tag{7.2}$$

Moreover, when $\boldsymbol{\psi}$ has the form (6.5), $\nabla_1\boldsymbol{\psi}(\boldsymbol{x},\boldsymbol{y}) = \nabla_1\boldsymbol{\psi}(\boldsymbol{0},\boldsymbol{y})$ for all $\boldsymbol{x} \in \mathbb{R}^3$, and the set of transformations of the form $\nabla_1\boldsymbol{\psi}(\boldsymbol{0},\ \boldsymbol{y})$ forms a group $\boldsymbol{F_0}$.

However, once $\boldsymbol{\psi}$ is specified, and one supposes that $L(\boldsymbol{0}) = \mathcal{I}$ say, the range of the field $L(\cdot)$ is known and is not generally the whole of $M_{3\times3}^+$. Therefore the construction outlined above needs to be modified a little if one supposes that strain energy functions of interest $\tilde{w}(\cdot, \mathcal{S})$ are defined over $M_{3\times3}^+$.

- The objective, given $L \in M_{3\times3}^{+}$, $\mathcal{S}$ satisfying the (analogue of) the Jacobi identity, and a point $e \in \mathbb{R}^3$, is to construct right invariant fields with $\tilde{\ell}_a(e) = Le_a$ and corresponding group composition function affine, call it $\tilde{\psi}$. Then, bearing in mind Theorem 3, the group $F_e = \left\{ \nabla_1 \tilde{\psi}(e, y);\ y \in \mathbb{R}^3 \right\}$ is a commutative group of linear transformations. Finally we will investigate the assumption that

$$w(L, \mathcal{S}) = w(\bar{F}L, \mathcal{S}), \quad \bar{F} \in F_e, \tag{7.3}$$

where $\mathcal{S}$ is the ddt. obtained from the right invariant fields.

So we propose the following general construction, which is analogous but not identical to that in Section 2;

- Let ψ be defined by (6.5), and construct fields $\ell_a(\cdot)$ with $\ell_a(0) = e_a$. Define the elastic deformation $y : \mathbb{R}^3 \to \mathbb{R}^3$ by

$$y(x) = Fx + e \tag{7.4}$$

where $Fe_a = Le_a$. Let $\left\{ \tilde{\ell}_a(\cdot),\ \mathbb{R}^3 \right\}$ be the state elastically related to $\left\{ \ell_a(\cdot),\ \mathbb{R}^3 \right\}$ by the deformation y, so

$$\tilde{\ell}_a(y(x)) = F\ell_a(x),\ \tilde{\ell}_a(e) = F\ell_a(0) = Fe_a = Le_a. \tag{7.5}$$

The composition function for this state is given by

$$\tilde{\psi}(y(x), y(u)) = y(\psi(x, u)), \tag{7.6}$$

and one checks that $y(0) = e$ acts as the group identity for this composition function. Therefore the relevant symmetries of the energy density are

$$F_e = \left\{ \nabla_1 \tilde{\psi}(e, y),\ y \in \mathbb{R}^3 \right\}$$

and

$$w(L, \mathcal{S}) = w(\tilde{F}L, \mathcal{S}), \quad \tilde{F} \in F_e. \tag{7.7}$$

One calculates from (7.6) that

$$\begin{aligned}
\tilde{\psi}(Fx + e,\ Fu + e) &= F\left(u + e^{-u_3 C} x \right) + e \\
&= (Fu + e) + Fe^{-u_3 C} x,
\end{aligned} \tag{7.8}$$

so that

$$\tilde{\psi}(\tilde{x}, \tilde{u}) = Fe^{-\{F^{-1}(\tilde{u}-e)\}_3 C}\left(F^{-1}(\tilde{x} - e) \right), \tag{7.9}$$

and

$$\nabla_1 \tilde{\psi}\, (\boldsymbol{e}, \tilde{\boldsymbol{u}}) = F e^{-\{F^{-1}(\tilde{\boldsymbol{u}} - \boldsymbol{e})\}_3 C} F^{-1}. \tag{7.10}$$

Note that $\{F^{-1}(\tilde{\boldsymbol{u}} - \boldsymbol{e})\}_3$ ranges over all of $\mathbb{R}^3$, as $\tilde{\boldsymbol{u}}$ varies in $\mathbb{R}^3$. Define the commutative group

$$G = \left\{ g : g = e^{tC}, t \in \mathbb{R} \right\}. \tag{7.11}$$

Then

$$F_{\boldsymbol{e}} = FGF^{-1}, \tag{7.12}$$

and this is the group that we propose should be adopted in (7.3). Note however that $F = L$ (see after (7.4)). Therefore, condition (7.3) becomes

$$w(L, \mathcal{S}) = w(Lg, \mathcal{S}) \quad g \in G. \tag{7.13}$$

In this form, L can be any element of $M_{3 \times 3}^+$, G is a fixed group determined by the ddt., see (7.11), and equation (7.13) is entirely analogous to the usual definition of material symmetry in nonlinear elasticity theory – the only difference being that $\mathcal{S}$ enters as a parameter, and that the symmetry group is determined by $\mathcal{S}$. Thus the 'canonical state' that has been constructed acts as 'reference configuration', and the symmetries of that configuration (according to our assumptions) 'act on the right' in the usual way.

Finally, there is one further issue to consider – we ask if there is any elastic deformation which preserves the form of the canonical states. For if there were a nontrivial elastic deformation such that the expression for the composition function in the new coordinates were unchanged by the deformation the construction that we have prescribed would seem not to be well-defined. Therefore we ask if there is an elastic deformation $\boldsymbol{y}$ such that

$$\boldsymbol{y}\left(\boldsymbol{u} + e^{-u_3 C}\boldsymbol{x}\right) = \boldsymbol{y}(\boldsymbol{u}) + e^{-y_3(\boldsymbol{u})C}\boldsymbol{y}(\boldsymbol{x}), \tag{7.14}$$

with

$$\boldsymbol{\ell}_a(\boldsymbol{0}) = \boldsymbol{\ell}_a\left(\boldsymbol{y}(\boldsymbol{0})\right) = \nabla\boldsymbol{y}(\boldsymbol{0})\boldsymbol{\ell}_a(\boldsymbol{0}), \quad a = 1, 2, 3, \tag{7.15}$$

so that

$$\nabla\boldsymbol{y}(\boldsymbol{0}) = \mathcal{I}. \tag{7.16}$$

Putting $\boldsymbol{x} = 0$ in (7.14) we get

$$\boldsymbol{y}(\boldsymbol{0}) = \boldsymbol{0}. \tag{7.17}$$

Differentiating (7.14) with respect to $\boldsymbol{x}$, putting $\boldsymbol{x} = \boldsymbol{0}$, and using (7.16),

$$\nabla\boldsymbol{y}(\boldsymbol{u})e^{-u_3 c} = e^{-y_3(\boldsymbol{u})C}\nabla\boldsymbol{y}(\boldsymbol{0}) = e^{-y_3(\boldsymbol{u})C}, \tag{7.18}$$

so
$$\nabla \boldsymbol{y}(\boldsymbol{u}) = e^{(u_3 - y_3(\boldsymbol{u}))C}. \tag{7.19}$$

In particular, (7.19) gives

$$(\nabla \boldsymbol{y}(\boldsymbol{u}))^T \boldsymbol{e}_3 = \nabla y_3(\boldsymbol{u}) = e^{(u_3 - y_3(\boldsymbol{u}))C^T} \boldsymbol{e}_3 = \boldsymbol{e}_3, \tag{7.20}$$

since $e^{(u_3 - y_3(\boldsymbol{u}))C^T}$ has the block structure (6.3). So $y_3 = u_3$, using (7.17), and (7.19) gives $\nabla \boldsymbol{y}(\boldsymbol{u}) = \mathcal{I}$. Therefore there is no non trivial elastic deformation which leaves the form of the canonical state (or composition function) invariant, and the construction that we have proposed is well-defined.

8. Representations

Here we catalogue various representations of energy functions which satisfy (7.13) and also a condition of objectivity, namely that

$$w(L, \mathcal{S}) = w(RL, \mathcal{S}), \quad R \text{ orthogonal.} \tag{8.1}$$

Equation (8.1) implies that $w(\cdot, \mathcal{S})$ can be written as

$$w(L, \mathcal{S}) = w'(\mathbb{C}, \mathcal{S}), \quad \mathbb{C} = L^T L, \tag{8.2}$$

and (7.13) then gives that

$$w'(\mathbb{C}, \mathcal{S}) = w'(g^T \mathbb{C} g, \mathcal{S}), \quad g \in G. \tag{8.3}$$

Again, (8.3) is a restriction entirely analogous to material symmetry restrictions imposed in nonlinear elasticity, the only difference being the parameter $\mathcal{S}$, and choice of group G. Note that G depends on $\mathcal{S}$ only through the composition function $\boldsymbol{\psi}$, and therefore that G depends only on the equivalence classes of $\mathcal{S}$ that were catalogued above. Below we give examples of the solution of (8.3) (for $w'(\cdot, \mathcal{S})$) for some equivalence classes with $\mathcal{S}$ singular.

(i) $\mathcal{S} = 0, \boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x} + \boldsymbol{y}, \ \nabla_1 \boldsymbol{\psi}(\boldsymbol{0}, \boldsymbol{x}) = \mathcal{I}, \quad G = \{\mathcal{I}\}.$

In this case (8.3) gives no restrictions on $w'(\cdot, \mathcal{S})$. Note that the usual discrete crystallographic groups derive from more information than is presumed in this paper – that the crystal determined by "initial values" $\boldsymbol{\ell}_a$, $\mathcal{S} = 0$, is in fact a perfect lattice determined by an equivalence class of basis vectors, amongst them the basis $\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}$, and that the corresponding response function depends on the lattice, rather than on the basis chosen to describe it. Cermelli and Parry [3] present a discussion of the relationship

between symmetries deriving from a generalised change of basis in (some) defective crystals, and the kind of symmetries that are assumed in this paper (see also the 'further motivation' section of this paper).

(ii) $\mathcal{S}_{12} = 1$, $C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, $e^{tC} = \begin{pmatrix} e^t & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{pmatrix}$. So (7.13) gives, with

$\mathbb{C} = L^T L = \begin{pmatrix} A & a & b \\ a & B & c \\ b & c & C \end{pmatrix}$, that

$$w'(A, B, C, a, b, c) = w'(t^2 A, B, C, ta, tb, c).$$

With fixed B, C, c, changing $A \to \frac{1}{2}\ln A$, $a \to \ln a$, $b \to \ln b$, putting $w'(A, B, C, a, b, c,) = w''(\frac{1}{2}\ln A, \ln a, \ln b)$,

$$\begin{aligned} w''(\tfrac{1}{2}\ln A, \ln a, \ln b) &= w''(\tfrac{1}{2}\ln A + \ln t, \ln a + \ln t, \ln b + \ln t) \\ &= w''(0, \ln a - \tfrac{1}{2}\ln A, \ln b - \tfrac{1}{2}\ln A) \\ &= w'\left(1, B, C, \frac{a}{\sqrt{A}}, \frac{b}{\sqrt{A}}, c\right) \end{aligned}$$

and this is the general representation of the solution.

(iii) For example $\mathcal{S}_{11} = \mathcal{S}_{22} = 1$. $C = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, $e^{tC} = $

$\begin{pmatrix} \cos t & -\sin t & 0 \\ \sin t & \cos t & 0 \\ 0 & 0 & 1 \end{pmatrix}$. So (7.13) gives that w is transversely isotropic with distinguished axis e_3, and one may read off the appropriate representation from, say, Green and Adkins [10].

9. Summary

One may summarise the procedure above rather quickly, in hindsight, and remark that the motivation for regarding the derived symmetry properties as appropriate is analogous to that presented in section 2.

Thus the canonical procedure for constructing a state with starting point e (acting as group identity), given values L_0 of the frame at the point e, and given ddt. $\mathcal{S}$, is the following; define an elastic deformation y with gradient $F \equiv L_0$ by

$$y(x) = Fx + e, \quad \text{so} \quad y(0) = e. \tag{9.1}$$

Elastic deformation of the frame $L(\boldsymbol{x}) \equiv e^{x_3 C}$, (cf. Theorem 3), gives a frame $L'(\cdot)$ defined by

$$L'(F\boldsymbol{x} + \boldsymbol{e}) = Fe^{x_3 C}, \quad \text{or} \quad L'(\boldsymbol{y}) = Fe^{\{F^{-1}(\boldsymbol{y}-\boldsymbol{e})\}_3 C}. \tag{9.2}$$

So, equation (9.2) defines the general canonical state, whose symmetries we have investigated in the body of the paper. The composition function for state defined by $L(\cdot)$ is $\boldsymbol{\psi}(\boldsymbol{x}, \boldsymbol{u}) = \boldsymbol{u} + e^{u_3 C}\boldsymbol{x}$, so by (7.6), the composition function for state defined by $L'(\cdot)$ is

$$\boldsymbol{\psi}'(\boldsymbol{x}', \boldsymbol{u}') = \boldsymbol{u}' + Fe^{\{F^{-1}(\boldsymbol{u}'-\boldsymbol{e})\}_3 C}F^{-1}(\boldsymbol{x}' - \boldsymbol{e}). \tag{9.3}$$

Thus the symmetries of the state Σ' defined by starting values $\boldsymbol{e}, L_0$, and ddt. $\mathcal{S}$, are of the form $Fe^{tC}F^{-1}$, where $F \equiv L_0$.

The crucial point is this; that the state defined by the lattice vectors $(Fe^{tC}F^{-1})L'(\cdot)$ is a *translation* of the state defined by lattice vectors $L'(\cdot)$, and this is the motivation for asserting that (7.7), or equivalently (7.13), holds (since the energy density should be independent of the translations of the canonical state). To see this, define

$$\begin{aligned} L''(\boldsymbol{x}) &= Fe^{tC}F^{-1}L'(\boldsymbol{x}) \\ &= Fe^{tC}e^{\{F^{-1}(\boldsymbol{x}-\boldsymbol{e})_3\}C}, \end{aligned} \tag{9.4}$$

from $(9.2)_2$. But this can be rearranged as

$$L''(\boldsymbol{x}) = Fe^{\{F^{-1}(\tilde{\boldsymbol{x}}-\boldsymbol{e})_3 C}, \text{ when } \tilde{\boldsymbol{x}} = \boldsymbol{x} + tF\boldsymbol{e}_3. \tag{9.5}$$

So

$$L''(\boldsymbol{x}) = L'(\tilde{\boldsymbol{x}}) = L'(\boldsymbol{x} + tF\boldsymbol{e}_3), \tag{9.6}$$

i.e. the effect of the symmetry operation is to translate the fields which define the canonical state. Moreover the set of symmetries that relate to (7.7), $\{Fe^{tC}F^{-1}; \ t \in \mathbb{R}\}$, is independent of the starting point $\boldsymbol{e}$, it depends only on L_0 and $\mathcal{S}$. When reformulated as (7.13), the set of symmetries is $\{e^{tC}; \ t \in \mathbb{R}\}$, which depends only on $\mathcal{S}$.

Acknowledgements

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