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DISCRETE STRUCTURES IN CONTINUUM DESCRIPTIONS OF DEFECTIVE CRYSTALS

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Abstract. I discuss various mathematical constructions that combine together to provide a natural setting for discrete and continuum geometric models of defective crystals. In particular I provide a quite general list of 'plastic strain variables', which quantifies inelastic behaviour, and exhibit rigorous connections between discrete and continuous mathematical structures associated with crystalline materials that have a correspondingly general constitutive specification.

1. Introduction

The geometrical context of the work is a kinematical model of defective crystals that Davini proposed in 1986, [1]. In that model a crystal state Σ, in $\mathbb{R}^3$, is given by the prescription of three smooth linearly independent 'lattice vector' fields $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot)$ defined at each point of some region $\Omega \subseteq \mathbb{R}^3$.

He interpreted these vector fields as averages, 'over regions with diameters large compared to spacing between atoms', [2], of quantities obtained from a (discrete) microscopic configuration of atoms or other structural elements. Thus the lattice vector fields were to vary on a scale finer than that commonly associated with continuum mechanics, coarser than interatomic. This separation of scales was motivation for the presumption that, in general changes of crystal state, these vector fields may evolve independently of the macroscopic deformation of continuum mechanics, even though the particular changes of state where the macroscopic deformation does determine the changes in those fields are highlighted, conceptually, and given a special status in the subsequent analysis (c.f. the definition of elastic deformation of lattice vector fields, (2.2) below).

His intention was that the vector fields 'were to represent in some average sense properties of the lattice including occasional defects that may occur at the atomistic level ', [2].

A further important feature of this model was that only the fields of lattice vectors, and certain of their derivatives, were required for constitutive purposes − for example, continuum energy densities were to be determined by such

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fields, so that this finite set of fields was deemed to be sufficiently indicative for continuum purposes of the relevant discrete microscopic configuration of atoms (say). This implies, in particular, that only the 'current 'set of vector fields is required, to determine constitutive functions, and there is no associated 'reference'or 'intermediate 'configuration, a priori.

With these assumptions, which are reminiscent of early molecular theories of elasticity, [3], [4], it became necessary to correlate features of the model with notions that are found useful in later theories of continuous distributions of dislocations, [5], [6], and in engineering plasticity theories [7, 8]. This was done by investigating and emphasizing the roles that the Burgers vectors, the dislocation density and torsion tensors, and rigorous versions of elastic-plastic decomposition, play in the analysis of Davini's kinematical model. In fact, there is one central question in that analysis which leads directly to the importance of the above notions − it is very simply stated: if two crystal states are given, that is if two sets of vector fields (defined over different regions of $\mathbb{R}^3$) are given, then how does one decide if there is a macroscopic deformation, mapping one region to the other, which also maps one set of fields to the other. To discuss this question, it was necessary to consider quantities of higher order (in the derivatives of the lattice vector fields) than the Burgers vector, dislocation density tensor, etc., though it was shown that only a finite number of such objects were necessary for the results obtained − these quantities are certain directional derivatives of the dislocation density tensor.

In summary, the model has many points of contact with other continuum models of materials which allow inelastic behaviour, the central geometrical object (a set of vector fields) is rather simple, at first glance, and decompositions of changes of crystal states into elastic and inelastic parts are derived results, based on the geometry of the vector fields (rather than constitutive hypotheses).Thus the model has many advantages, but:

(1) The process of averaging, by which smooth vector fields are derived from a discrete microscopic configuration with 'occasional defects ', is not made precise in [1],[2], nor in any related work that I know of;
(2) The higher order quantities which are important in order to make connections with, for example, the (ad hoc) elastic-plastic decompositions of plasticity theory, have had no compelling geometrical interpretation, to date, by way of contrast with the Burgers vector, dislocation density tensor, etc.

I address these two limitations in this paper. To be precise regarding (i), though, I do not propose any particular averaging process, nor make any presumption regarding the density or distribution of defects, rather I consider

a 'converse 'approach − that is, I ask if any discrete set of points is 'naturally 'associated with a given set of lattice vector fields. In fact the question has to be more specific than this, if there is to be any mathematical resolution of the issue, and it is made specific by constraining the vector fields in a manner that I outline towards the end of this introduction.

The final result, regarding (i), is that there is indeed a set of points associated with any set of vector fields so constrained, and that such sets of points have a regularity that derives from a continuous (Lie) group structure. Also, the dimension of the group (i.e. the number of real parameters required to specify a general group element) depends on the number of 'higher order quantities ', c.f. (ii), involved in defining the set of vector fields. Thus, for example, when the vector fields are constant in $\mathbb{R}^3$, so that the dislocation density tensor is zero, the relevant continuous group corresponds to translation in $\mathbb{R}^3$ and the corresponding set of points is a perfect lattice. When the vector fields are such that only the dislocation density tensor is required, for the purposes sketched in (ii), the relevant continuous group is three dimensional (but not a group of translations) and the corresponding set of points is not generally a perfect lattice (it may be a collection of perfect lattices, for example). When higher order quantities are required , for the purposes of (ii), the relevant continuous group has dimension strictly greater than three, and points in $\mathbb{R}^3$ are obtained by projection (to $\mathbb{R}^3$) of a corresponding 'regular 'higher dimensional set of points. So, one constructs a hierarchy of continuous and discrete structures for each set of vector fields satisfying the constraints.

This result, which is based on a theorem [9] whose relevance in this context was highlighted by Elzanowski and Preston in [10], allows one to interpret the geometrical information that is implicit when a list of constitutive variables of a certain general type is prescribed: suppose that *values* of the dislocation density tensor and a finite number of its directional derivatives are prescribed, and that these values are consistent with a set of lattice vector fields constrained as above. Then there is a related continuous group structure whose dimension is determined by the order of that set of derivatives of the vector fields, together with an associated 'regular '(possibly discrete) set of points. Thus the 'local '(continuous) structure determined by point values of the dislocation density tensor and some of its derivatives is a certain Lie group.

So it should be possible, in due course, to construct an 'atlas 'of discrete structures of this type − then, given a microscopic configuration of structural elements in some dynamically stable amorphous solid, for example, one might identify the particular chart(s) in that atlas that correspond to the observed configuration, and so determine a list of constitutive variables appropriate for the continuum mechanical modelling of such materials. This is the sense in which the present approach is converse to Davini's original suggestion. Also

the scheme fits with the mechanics of complex materials, to the extent that there is a local microstructure at each material point (at each material point there is a Lie group , and possibly discrete set of group elements, determined by point values of the constitutive variables).

Regarding point (ii) and the specific constraints on the set of vector fields mentioned above, it is shown below (c.f.(2.19)) that there a connection between the directional derivatives of the dislocation density tensor and quantities obtained by *iteration* of the Burgers vector construction. The specific constraints on the vector fields, needed in order to justify the remarks of the last two paragraphs, loosely stated, are that only a finite number of iterations of the Burgers vector construction are required in order that iterations of all orders be determined. By virtue of connections such as (1.19) below, the constraint can be recast in terms of directional derivatives of the dislocation density tensor, giving that directional derivatives of all orders are to be determined by lower order terms in a certain way. Finally, regarding (ii), since (1.19) generalizes to give connections between higher order directional derivatives of the dislocation density tensor and successive iterations of the Burgers vector construction, we have the required geometrical interpretation of the higher order terms.

In the next section I outline the nature of the mathematical apparatus that is required in order to justify the above remarks, before giving more detail in the later sections.

2. Outline

Let $\{\boldsymbol{l}_a(\cdot)\}$ denote the set of three linearly independent fields $\boldsymbol{l}_1(\cdot), \boldsymbol{l}_2(\cdot), \boldsymbol{l}_3(\cdot)$, so that the crystal state Σ is defined by

$$\Sigma \equiv \{\{\boldsymbol{l}_a(\cdot)\}\,;\Omega\}\,. \tag{2.1}$$

An elastic deformation of Σ is a smooth invertible mapping $\boldsymbol{u} : \Omega \to \boldsymbol{u}(\Omega) \subseteq \mathbb{R}^3$, such that the fields $\{\boldsymbol{l}_a(\cdot)\}$ are transformed to fields $\{\tilde{\boldsymbol{l}}_a(\cdot)\}$ defined on $\boldsymbol{u}(\Omega)$, where

$$\tilde{\boldsymbol{l}}_a\left(\boldsymbol{u}(\boldsymbol{x})\right) \equiv \nabla\boldsymbol{u}(\boldsymbol{x})\boldsymbol{l}_a(\boldsymbol{x}),\ a = 1, 2, 3,\ \boldsymbol{x} \in \Omega. \tag{2.2}$$

The crystal state

$$\tilde{\Sigma} \equiv \{\{\tilde{\boldsymbol{l}}_a(\cdot)\}; \tilde{\Omega}\}. \tag{2.3}$$

is said to be elastically related to Σ when (2.2) holds and $\tilde{\Omega} = \boldsymbol{u}(\Omega)$, and vice versa via $\boldsymbol{u}^{-1}(\cdot)$.

Mathematical quantities calculated from the lattice vector fields and their derivatives of any order which are both (i) additive over disjoint subregions of Ω, and (ii) invariant under elastic deformation, are said to be 'measures of defectiveness'. These quantities are represented by
integrals over curves, surfaces and volumes, by virtue of the additivity requirement, and corresponding densities include the Burgers vectors and the dislocation density tensor. Note that I shall refer to corresponding *scalar* densities as 'elastic invariants' — each component of the dislocation density (defined below) is an elastic invariant, but the Burgers vectors are not, for example. The dislocation density 'tensor' (so-called) consists of nine elastic invariants $S_{ab}, a, b = 1, 2, 3$ defined as follows:

$$S = (S_{ab}) \equiv \left(\frac{\nabla \wedge \boldsymbol{d}_a \cdot \boldsymbol{d}_b}{n}\right), \tag{2.4}$$

where the smooth linearly independent fields $\boldsymbol{d}_1(\cdot), \boldsymbol{d}_2(\cdot), \boldsymbol{d}_3(\cdot)$ are dual to the lattice vector fields;

$$\boldsymbol{l}_a(\boldsymbol{x}) \cdot \boldsymbol{d}_b(\boldsymbol{x}) = \delta_{ab}, \quad \boldsymbol{l}_a(\boldsymbol{x}) \otimes \boldsymbol{d}_a(\boldsymbol{x}) = \text{ identity}, \quad \boldsymbol{x} \in \Omega, \tag{2.5}$$

where δ_{ab} is the Kronecker delta, and $n(\cdot)$ is defined by

$$n \equiv \boldsymbol{d}_1 \cdot \boldsymbol{d}_2 \wedge \boldsymbol{d}_3. \tag{2.6}$$

Each of the quantities $(\nabla \wedge \boldsymbol{d}_a)(\cdot)$ is referred to as a 'Burgers vector' field.

Now the following observation is central to the discussion: if $\vartheta(\cdot)$ is any elastic invariant, so are $(\boldsymbol{l}_a \cdot \nabla\vartheta)(\cdot)$, $a = 1, 2, 3$. Thus, all directional derivatives of S, of any order, are also elastic invariants, so that there is an infinite number of such objects.

The particular elastic invariants

$$S, \quad \boldsymbol{l}_a \cdot \nabla S, \tag{2.7}$$

will be of fundamental significance, subsequently.

The **first theme** to be discussed in the paper is the following: give a finite functional basis for the set of elastic invariants, and a similar basis for the measures of defectiveness. (I'll be precise about what is meant by a functional basis later). These tasks were addressed in [11, 12, 13, 14] , and I note that some of the results relevant to the first task can be read in terms of, and understood by means of, Cartan's theory of equivalence of vector fields, as set out by Olver in [15].

The **second theme** (there are five in all) relates to the fact that two distinct crystal states may not be elastically related to one another even if they have identical measures of defectiveness. I say that, as in [11, 12], two crystal states are related by (implicitly non-trivial) *neutral deformation* in that case, and remark that the corresponding changes of state can be interpreted in terms of rearrangements of vector fields, or 'slip'. The equations that determine whether or not a crystal state Σ (c.f. (2.1)) allows neutral deformation are partial differential equations for lattice vector fields $\left\{\boldsymbol{l}'_a(\cdot)\right\}$ in a crystal state also defined on $\Omega \subseteq \mathbb{R}^3$,

$$\Sigma' \equiv \left\{\left\{\boldsymbol{l}'_a(\cdot)\right\}, \Omega\right\}. \tag{2.8}$$

One solution of these partial differential equations is $\{\boldsymbol{l}_a(\cdot)\}$, neutral deformations exist if there is a solution $\left\{\boldsymbol{l}'_a(\cdot)\right\} \neq \{\boldsymbol{l}_a(\cdot)\}$.

The interpretation of neutral deformations as slip, [11, 12], suggests that states which allow neutral deformation are important from the point of view of the theory of plasticity, or engineering theories of inelastic behaviour, and so I confine attention *throughout* to such states. This permits us, it turns out, to focus on a list of elastic invariants that includes only some of the lower order elements from the general functional basis for the set of all elastic invariants. Also this restriction gives more information about the lattice vector fields than would otherwise be the case, of course, and it makes the subsequent mathematics more tractable. Note that the restriction does not play a direct role in Cartan's view of the geometry, nor in continuum theories of continuous distributions of dislocations, though the phenomenological theories do give slip a fundamental ad hoc status (if that is not a contradiction in terms).

Next I regress a little and return to ask what it means for a list of elastic invariants to be a functional basis, in general and in the case where crystal states allow neutral deformation, so that one aspect of the significance of (2.7) is evident. First it is clear, since we are working in $\mathbb{R}^3$, that there can be at most three independent elastic invariants

(for if there is a set of three invariants ν_1, ν_2, ν_3 such that the corresponding three gradients form a set of linearly independent vectors at each point $\boldsymbol{x}$ of Ω, then one can invert to write $\boldsymbol{x} = \boldsymbol{x}(\nu_1, \nu_2, \nu_3)$, and so use those three invariants as a system of coordinates with which to specify the dependence of any other invariant on position in $\mathbb{R}^3$). Any such set of three elastic invariants must be included in the set of all directional derivatives of S up to and including second order. This does not imply that ν_1, ν_2, ν_3 is a functional basis of the set of all elastic invariants, though, for one cannot calculate invariants of any higher order explicitly, given ν_1, ν_2, ν_3. However it is enough (in order to provide a functional basis for all invariants) to add the set of third order invariants to those of lower order. For if (any) third order invariant I is known, then by the above remarks it can be written in the form $I = I(\nu_1, \nu_2, \nu_3)$, and then

$$\boldsymbol{l}_a \cdot \nabla I = \frac{\partial I}{\partial \nu_i}(\boldsymbol{l}_a \cdot \nabla \nu_i), \quad a = 1, 2, 3, \tag{2.9}$$

using the summation convention. Since $\boldsymbol{l}_a \cdot \nabla \nu_i$ is an invariant of order 3 at most, $a, i = 1, 2, 3$, it can be written as a (known) function of ν_1, ν_2, ν_3, and since $I = I(\nu_1, \nu_2, \nu_3)$ is known, so is $\frac{\partial I}{\partial \nu_i}$, $i = 1, 2, 3$. All fourth order invariants have the form $\boldsymbol{l}_a \cdot \nabla I$, and so all fourth order invariants are also known, from (2.9). Iterating, one can find all invariants, of arbitrary order, explicitly. This implies that

$$\text{the set of all directional derivatives of } S \text{ of order } \leq 3, \tag{2.10}$$

is a functional basis of the set of all elastic invariants ('plastic strain' variables), in the sense that all other elastic invariants may be found if these particular invariants are prescribed in a domain $\Omega \subseteq \mathbb{R}^3$.

In the case of crystal states that allow neutral deformations, it turns out that, if there is a non-constant elastic invariant, ν say, then all other invariants may be expressed in terms of ν. This invariant ν may be taken as some element of (S_{ab}) without loss of generality, and in the case that all first order invariants are known in terms of ν, all higher order invariants may be found explicitly. Thus

$$\text{the set of all directional derivatives of } S \text{ of order } \leq 1, \tag{2.11}$$

is a functional basis of the set of all elastic invariants, in this case, c.f. (2.7). In the case that

$$\text{all elements of } S, \tag{2.12}$$

are constant in Ω, all the other elastic invariants are zero.

Thus the list (2.7) is a functional basis of the set of all elastic invariants, in the case that the crystal state allows neutral deformation.

Note that the invariants of (2.7) are not arbitrary — they are subject to two constraints deriving from the identities

$$0 = \nabla \cdot (\nabla \wedge \boldsymbol{d}_a) = \nabla \cdot (nS_{ab}\boldsymbol{l}_b),\ \mathbf{0} = \nabla \wedge (\nabla\nu) = \nabla \wedge \{(\boldsymbol{l}_a \cdot \nabla\nu)\boldsymbol{d}_a\}\,. \quad (2.13)$$

These constraints are the only constraints on those variables — this will be dealt with in section 5.

In section 5, I turn to the **third theme**, which is the connection between the continuum description of the crystal and the theory of Lie groups. The connection is approached, first of all, by noting from [13, 14] that the Lie brackets of pairs of lattice vector fields, defined by

$$\boldsymbol{L}_1 \equiv [\boldsymbol{l}_2, \boldsymbol{l}_3] \equiv (\boldsymbol{l}_3 \cdot \nabla)\boldsymbol{l}_2 - (\boldsymbol{l}_2 \cdot \nabla)\boldsymbol{l}_3, \quad (2.14)$$

for example, are connected to the dislocation density tensor by:

$$S_{ab} = \boldsymbol{L}_b.\boldsymbol{d}_a,\ \text{or}\ S_{ab}\boldsymbol{l}_a = \boldsymbol{L}_b, \quad a, b = 1, 2, 3. \quad (2.15)$$

In the simplest case, where $S = (S_{ab})$ is constant in Ω, these nine constants are related to the structure constants C_{ijk} of a three dimensional Lie algebra $\mathfrak{g}$ via

$$\varepsilon_{jkl}S_{ij} = C_{ikl}, \quad i, k, l = 1, 2, 3, \quad (2.16)$$

where ε_{ijk} are components of the permutation symbol. Also, there is a set of vector fields (again denoted) $\{\boldsymbol{l}_a(\cdot)\}$ defined on the corresponding three dimensional Lie group G, with composition function $\boldsymbol{\chi} : G \times G \to G$, that satisfies (2.4) above and also

$$\boldsymbol{l}_a\left(\boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y})\right) = \nabla_1\boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{l}_a(\boldsymbol{x}), \quad a = 1, 2, 3,\ \boldsymbol{x}, \boldsymbol{y} \in G, \quad (2.17)$$

where $\nabla_1\boldsymbol{\chi}(\cdot, \cdot)$ denotes the gradient of $\boldsymbol{\chi}$ with respect to its first argument. According to (2.17), the vector fields $\{\boldsymbol{l}_a(\cdot)\}$ are *right invariant* with respect to group multiplication (i.e. by $\boldsymbol{y} \in G$ on the right).

One should not dismiss (2.17) as a mathematical nicety for it represents the answer to a long standing question in the theory of defects, which is how crystals 'fit together' when there are defects present. Equation (2.17) tells us that, in the case $S =$ constant (so that there is a uniform distribution of defects, in some sense), there is an explicit self-similarity of the lattice vector fields — (2.17) states that, for any given $\boldsymbol{y}$, there is an elastic deformation $\boldsymbol{x} \to \boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y})$ which maps lattice vector fields in a neighbourhood of (any) $\boldsymbol{x}_0$ to lattice vector fields in a corresponding neighbourhood of $\boldsymbol{\chi}(\boldsymbol{x}_0, \boldsymbol{y})$ (and since G is a group, the point $\boldsymbol{\chi}(\boldsymbol{x}_0, \boldsymbol{y})$ may be considered arbitrary, by choice of $\boldsymbol{y}$).

That is, (2.17) is (2.2) with $\boldsymbol{u}(\boldsymbol{x}) \equiv \boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y})$, and $\Sigma = \tilde{\Sigma}$. In brief, 'Σ is elastically related to itself, locally'.

In the sequel, we shall arrive at a result analogous to (2.17) in the case that S is not constant.

I take the point of view that the construction that leads to (2.17), in the case that S is constant in Ω, relates to a continuum where the list of constitutive variables includes a dependence on S, but that there is no dependence on $\{\boldsymbol{l}_a \cdot \nabla S\}$, nor any higher order directional derivatives of S, i.e. the appropriate list of plastic strain variables is (2.12). The following remarks are a generalization of this perspective, to include higher order directional derivatives of S. First, though, in order to progress, one has to recast these higher order directional derivatives into a more algebraic form, and this reformulation is one of the main ideas in the paper.

So what is the appropriate mathematical structure in the case that the constitutive variables include the 'plastic strain' variables in (2.11) - then S is non constant because $\boldsymbol{l}_a \cdot \nabla S \neq 0$, $a = 1, 2, 3$, in general? To begin to get at the connection, note first that, from the definition (2.14) of the Lie bracket,

$$[\phi \boldsymbol{l}_a, \boldsymbol{l}_b] = \phi[\boldsymbol{l}_a, \boldsymbol{l}_b] + (\boldsymbol{l}_b \cdot \nabla \phi)\boldsymbol{l}_a, \quad a, b = 1, 2, 3, \tag{2.18}$$

which holds for all functions $\phi : \mathbb{R}^3 \to \mathbb{R}$ but in particular when ϕ is a function of the directional derivatives of S of any order. Putting $\phi = S_{ac}$ and using $(2.15)_2$ we have

$$[\boldsymbol{L}_c, \boldsymbol{l}_b] = S_{ac}[\boldsymbol{l}_a, \boldsymbol{l}_b] + (\boldsymbol{l}_b \cdot \nabla S_{ac})\boldsymbol{l}_a, \quad b, c = 1, 2, 3. \tag{2.19}$$

Recall that $\boldsymbol{L}_1 = [\boldsymbol{l}_2, \boldsymbol{l}_3]$, etc., so the left side of (2.19) consists of terms such as $[[\boldsymbol{l}_1, \boldsymbol{l}_2], \boldsymbol{l}_3]$ — I'll call terms of that form 'nested' Lie brackets of order 3, $[\boldsymbol{l}_2, \boldsymbol{l}_3]$ a 'nested' Lie bracket of order 2, and for semantic convenience $\boldsymbol{l}_1$ a 'nested' Lie bracket of order 1. With this jargon in place, $(2.15)_2$, gives the nested Lie brackets of order 2 in terms of those order 1, (2.19) gives those of order 3 in terms of those of orders 1 and 2. In particular, (2.19) is a relation between nested Lie brackets of orders $3, 2, 1$ and the coefficients in that relation are elastic invariants that appear in the list (2.11), or (2.7). Also, $(2.15)_1$ gives S in terms of the nested brackets of order $1, 2$, (2.19) can be rearranged to give $\{\boldsymbol{l}_a \cdot \nabla S\}$ in terms of nested brackets of orders ≤ 3.

So if the list of constitutive variables includes a dependence on S and $\boldsymbol{l}_a \cdot \nabla S$, but on no higher derivatives of S, then that list of variables can be recast in terms of nested Lie brackets of order ≤ 3. To proceed, in this case, I follow [10], and make an *assumption*: it is that the nested brackets of orders ≤ 2 provides a basis for the nested brackets of order 3 — this amounts to a constraint on the elastic invariants additional to those that derive from (2.13) (in fact it implies that one of those two constraints is satisfied).

The assumption implies that nested brackets of all orders are determined as linear combinations of $\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}$, so we have a Lie algebra with basis included in the set $\{\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}\}$ — Elzanowski and Preston call this the *lattice algebra* derived from the lattice vector fields, and note that [9] gives the existence of a Lie group G (of dimension higher than the number of lattice vectors in the case $\nabla S \neq 0$) with corresponding Lie algebra $\mathfrak{g}$ homomorphic to the lattice algebra. We shall see later how the lattice vector fields are related to objects in G. This procedure gives the appropriate mathematical structure in the case that the constitutive variables include those listed in (2.11), and the assumption is readily generalized to include the case where the list of constitutive variables includes higher order directional derivatives of S.

Note that if the third order brackets are known in terms of a linear (i.e. constant coefficient) combination of lower order brackets, then in particular one can also calculate the 4^{th} order brackets in terms of a linear combination of lower order brackets, etc.

The **final two themes** focus on discrete structures that are associated with the continuum models above. In section 6 I deal with the case that S is constant, where the constitutive variables are $\{\boldsymbol{l}_a\}, S$ or equivalently $\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}$, and where material points can be associated with a three dimensional Lie group G. Using properties of right invariant fields, I motivate the assertion that the relevant structures are discrete subgroups of G. (Note the analogous result in the case $S = 0$ — the only discrete subgroups of $\mathbb{R}^3$, viewed as a Lie group with addition as group operations, are the perfect lattices, [16]). I summarize the procedure for a particular S and recall results which relate symmetries of discrete subgroups D so obtained with symmetries of the ambient Lie group G.

In section 7, I explore the case where $\nabla S \neq 0$. To simplify matters a little, I consider the case where the crystal state corresponds to the prescription of just two lattice vector fields defined on a region $\Omega \subseteq \mathbb{R}^2$, and I continue to require that the crystal state allows neutral deformations. Recall that, in the case $\nabla S \neq 0$, the relevant Lie group is of a dimension greater that the number of linearly independent lattice vector fields — I make a particular choice of lattice vectors such that the lattice algebra has dimension 3, in fact I make a choice such that the corresponding three dimensional Lie group is isomorphic to a group used in section 6, whose discrete subgroups are described in that section. I show how this 'three dimensional' discrete structure projects to the lower dimensional 'base', $\mathbb{R}^2$, via a certain group action $\lambda : G \times \mathbb{R}^2 \to \mathbb{R}^2$.

Finally, I summarize the work and indicate how it may be extended and improved.

3. Measures of defectiveness, elastic invariants

In [11, 12, 13, 14], Davini, Parry and Šilhavý searched for 'invariant integrals' in the context of the above kinematical model of defective crystals. These are circuit, closed surface or volume integrals (they are to mimic atomistic procedures: counting point defects in a given volume; counting edge dislocations crossing a given surface, for example) with integrands depending on the lattice vector fields and their derivatives of any order (succinctly, 'differential functions') which are functionals independent of elastic deformation. They are the 'measures of defectiveness' referred to in the introduction. Thus if $F_\Omega\left(\{\boldsymbol{l}_a(\cdot)\}\right)$ is any such functional, and fields $\{\tilde{\boldsymbol{l}}_a(\cdot)\}$ are defined by (2.2), then $F_{\tilde{\Omega}}(\{\tilde{\boldsymbol{l}}_a(\cdot)\}) = F_\Omega(\{\boldsymbol{l}_a(\cdot)\})$, with $\tilde{\Omega} = \boldsymbol{u}(\Omega)$. This search required discussion of the transformation properties, induced by (2.2), of the various derivatives of the lattice vector fields, of course — for example, $\det(\{\tilde{\boldsymbol{l}}_a\}) = \det(\nabla \boldsymbol{u}) \det(\{\boldsymbol{l}_a\})$ together with the definition $n = \boldsymbol{d}_1 \cdot \boldsymbol{d}_2 \wedge \boldsymbol{d}_3$ gives that $\int_V n dV = \int_{\tilde{V} \equiv \boldsymbol{u}(V)} \tilde{n} d\tilde{V}$ is an invariant integral (where $\det(\cdot)$ denotes the determinant and $V \subseteq \Omega$). In fact,

$$\int_V n \, dV, \int_V Sn \, dV, \int_{\mathcal{C}} \boldsymbol{d}_a \cdot \boldsymbol{dx} \text{ are invariant integrals,} \tag{3.1}$$

where $\mathcal{C}$ is a circuit, by recalling the definition of the dual fields $\{\boldsymbol{d}_a(\cdot)\}$ and the dislocation density S, and by calculating relevant transformation properties. As mentioned above, if ν is any elastic invariant (i.e. scalar differential function), then

$$\{(\boldsymbol{l}_a \cdot \nabla \nu)(\cdot)\} \text{ is a set of elastic invariant fields.} \tag{3.2}$$

As stated, if S has a least one non constant component, then there is in general an infinite number of elastic invariants, obtained from that particular component of S by successive directional differentiation. This implies that there is an infinite number of integral invariants too, because (for example)

$$\int_{\mathcal{C}} \nu \boldsymbol{d}_a \cdot \boldsymbol{dx} \text{ is an integral invariant if } \nu \text{ is any elastic invariant.} \tag{3.3}$$

It was shown in the above papers that there is a basis of integral invariants in the sense that if densities corresponding to the basis integral invariants are given, as fields in Ω, then the densities of all integral invariants can be determined. The basis integral invariants are:

$$\int_{\mathcal{C}} \nu \boldsymbol{d}_a \cdot \boldsymbol{dx}, \int_V \nu n \, dV : \quad \nu \in \{1, S, \{(\boldsymbol{l}_a \cdot \nabla S)\}\}. \tag{3.4}$$

4. Neutral deformations, the classifying manifold

It is a fundamental question, to ask if given two crystal states $\Sigma = \{\{\boldsymbol{l}_a(\cdot)\}\,;\Omega\}$, $\Sigma^* = \{\{\boldsymbol{l}^*_a(\cdot)\}\,;\Omega^*\}$ and a smooth mapping $\boldsymbol{u}$ with $\boldsymbol{u}(\Omega) = \Omega^*$ such that the basis integral invariants (3.4) match in the two states (in the obvious sense), whether or not Σ and Σ^* are elastically related to one another. This question can be reformulated by first mapping Σ^* elastically, via $\boldsymbol{u}^{-1}$, to a state $\Sigma' = \{\{\boldsymbol{l}'_a(\cdot)\}\,;\Omega\}$ — then the question reduces to asking whether or not the partial differential equations

$$\nabla \wedge \boldsymbol{d}_a = \nabla \wedge \boldsymbol{d}'_a,\ n = n',\ \nu = \nu',\ \nabla\nu \wedge \boldsymbol{d}_a = \nabla\nu \wedge \boldsymbol{d}'_a,\ \nu \in \{S, \{(\boldsymbol{l}_a \cdot \nabla S)\}\}\,, \tag{4.1}$$

have a unique solution for $\{\boldsymbol{l}'_a(\cdot)\}$, given $\{\boldsymbol{l}_a(\cdot)\}$ (use $\int_{\partial S} \boldsymbol{d}_a \cdot \boldsymbol{dx} = \int_S \nabla \wedge \boldsymbol{d}_a \cdot \boldsymbol{dS}$ to get $(4.1)_1$, etc.). The answer to this question is negative, in general — there are crystal states which are not elastically related to one another such that all the invariant integrals match in the two states, for some choice of the mapping $\boldsymbol{u}$. A simple example of the non-uniqueness of solutions of (4.1) is given in [12].

One implication of (4.1) is critically important for subsequent discussion. Suppose that (4.1) has a solution $\{\boldsymbol{l}'_a(\cdot)\} \neq \{\boldsymbol{l}_a(\cdot)\}$ and that ν is a non-constant element of $S = (S_{ab}(\cdot))$. Then by differentiating $(4.1)_3$ ((4.1) holds for all points in Ω), $\nabla\nu = \nabla\nu'$, and so from $(4.1)_4$, $\nabla\nu \wedge (\boldsymbol{d}_a - \boldsymbol{d}'_a) = \boldsymbol{0}$, $a = 1, 2, 3$. If ϑ is any of $\boldsymbol{l}_a \cdot \nabla S, a = 1, 2, 3$, we have from $(4.1)_3$ that $\nabla\vartheta \wedge (\boldsymbol{d}_a - \boldsymbol{d}'_a) = \boldsymbol{0}$, $a = 1, 2, 3$. Since $\boldsymbol{d}_a(\cdot) \neq \boldsymbol{d}'_a(\cdot)$ for some $a = 1, 2, 3$, it follows that $\vartheta = \vartheta(\nu)$, when (4.1) has non-unique solutions and S has a non-constant component. Furthermore, since $\boldsymbol{l}_b \cdot \nabla\vartheta = (\boldsymbol{l}_b \cdot \nabla\nu)\frac{d\vartheta}{d\nu}$, it follows that all second order directional derivatives of S are functions of ν, and by induction all directional derivatives of S have the same property.

As stated earlier, I consider only crystal states Σ where (4.1) has non-unique solutions for Σ' — I say that Σ admits *neutral deformations* in that case. Then

either $S =$ constant, or all elastic invariants are functions of one non-constant component of S (denoted ν). (4.2)

I recall the interpretation of neutral deformations as slip (rearrangements of lattice vector fields) in regions where the lattice vector fields are constant (see [11, 12]) and see the importance of slip in theories of inelastic behaviour as motivation to investigate the mathematical setting in some depth.

Now it is productive to consider some particular implications of equations (4.1), specifically the equations there that relate to the elastic invariants only:

$$\nu = \nu', \quad \nu \in \{S, \{\boldsymbol{l}_a \cdot \nabla S\}\}\,. \tag{4.3}$$

In the case that one component of S is non-constant, the elastic invariants $\{S, \{\boldsymbol{l}_a \cdot \nabla S\}\}$ are precisely those that appear in (2.11) — they are a functional basis for all elastic invariants. According to [11],[15], when (4.3) holds states Σ and Σ' are **locally elastically related** to one another (though not elastically related to one another, in general): states Σ and $\Sigma^* = \{\{\boldsymbol{l}^*_a(\cdot)\}; \Omega^*\}$ are locally elastically related if for each $\boldsymbol{x}_0 \in \Omega$, there exists a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_0}$ defined on a neighbourhood $N_{\boldsymbol{x}_0}$ of $\boldsymbol{x}_0$ in Ω, with $\boldsymbol{u}_{\boldsymbol{x}_0}(N_{\boldsymbol{x}_0}) \subset \Omega^*$ such that

$$\boldsymbol{l}^*_a\left(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})\right) = \nabla \boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}) \boldsymbol{l}_a(\boldsymbol{x}),\ a = 1, 2, 3, \boldsymbol{x} \in N_{\boldsymbol{x}_0}, \boldsymbol{x}_0 \in \Omega. \tag{4.4}$$

In the case where (4.3) holds, let $\boldsymbol{x}_0, \boldsymbol{x}'_0$ be any points such that $\nu(\boldsymbol{x}_0) = \nu'(\boldsymbol{x}'_0), \nu \in \{S, \{\boldsymbol{l}_a \cdot \nabla S\}\}$, (e.g., $\boldsymbol{x}_0 = \boldsymbol{x}'_0$ by (4.3)), then there exists a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_0}$ with $\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}_0) = \boldsymbol{x}'_0$ such that (4.4) holds with $\{\boldsymbol{l}^*_a(\cdot)\}$ replaced by $\{\boldsymbol{l}'_a(\cdot)\}$.

Now given a state $\Sigma = \{\{\boldsymbol{l}_a(\cdot)\}; \Omega\}$ admitting neutral deformations, with all elastic invariants functions of one non-constant invariant ν, one can introduce the one dimensional curve (in $\mathbb{R}^{9+27}$) which represents the values of the invariants $\{S, \{\boldsymbol{l}_a \cdot \nabla S\}\}$. So let

$$J \equiv \{\nu \in \mathbb{R} : \nu = \nu(\boldsymbol{x}),\ \boldsymbol{x} \in \Omega\}, \tag{4.5}$$

and define

$$C \equiv \left\{\boldsymbol{y} \in \mathbb{R}^{9+27}; \boldsymbol{y} = \{S(\nu), \{(\boldsymbol{l_a} \cdot \nabla S)(\nu)\}\},\ \nu \in J\right\}. \tag{4.6}$$

In Olver's terminology, the expression (4.6) represents the first order classifying set associated with the crystal state Σ. Assuming that this set is sufficiently well-behaved (all considerations in this paper are local, so this assumption is harmless), I'll call it (after Olver, again) the **classifying manifold** associated with Σ.

So, if crystal states Σ, Σ' are neutrally related (i.e. $\Sigma' \neq \Sigma$ solves (4.1), with Σ given), then in particular the corresponding classifying manifolds are identical, and Σ, Σ' are locally elastically related to one another.

In the case that S is constant the above still applies, it is just that in this case the classifying manifold is then the point $(S, \mathbf{0}) \in \mathbb{R}^{9+27}$. One also has the global statement (2.17), in addition to the result (4.4).

5. Constitutive hypotheses, Lie groups

There are two constraints on the classifying manifold, that I derive below. (In the case $S =$ constant, these two constraints reduce to (5.1) below, which is a form of the Jacobi identity). Given that caveat, the classifying manifold (4.6) quantifies all possible distributions of elastic invariants deriving from a crystal state that allows neutral deformations. One may consider a hierarchy of special cases:

(i) If $C = \{\mathbf{0} \in \mathbb{R}^{9+27}\}$, then S is identically zero and the crystal state consists of constant lattice vector fields, modulo elastic deformation. So, one imagines that a material where the constitutive variables do not include S or any of its directional derivatives is a material where $S = 0$ — one may then select a 'canonical' state where the lattice vector fields are constant from those elastically related to it;

(ii) At the next level of generality, if $C = \left\{(S, \mathbf{0}) \in \mathbb{R}^{9+27}\right\}$ with $S \in \mathbb{R}^9$, and with S satisfying the equation

$$S_{ai}(\varepsilon_{ijk}S_{jk}) = 0, \quad a = 1, 2, 3, \tag{5.1}$$

then I have indicated in the introduction that there is a Lie group G with right invariant lattice vector fields $\{\boldsymbol{l}_a(\cdot)\}$ satisfying (2.4). Any elastic deformation of the corresponding crystal state gives lattice vector fields which are right invariant with respect to a group isomorphic to G, with the same S. So one can imagine that a material where the constitutive variables include a dependence on S (satisfying (5.1)), but no dependence on higher derivatives of S, relates to crystal states corresponding to a particular choice of Lie group, chosen from those isomorphic to it. Any such crystal state has the self-similarity encapsulated by (2.17), at the continuum level;

(iii) In full generality (at least, for crystal states that allow neutral deformation), a list of constitutive variables that includes values of $S, \{\boldsymbol{l}_a \cdot \nabla S\}$ at some point $\boldsymbol{x}_0 \in \Omega$ determines a point of C, but no nontrivial arc of that curve. One needs to know in addition that the material is in a configuration such that S is a function of a single variable (i.e. that S is constant on surfaces $\nu =$ constant), with S and $\{\boldsymbol{l}_a \cdot \nabla S\}$ satisfying the constraints below, if one is to think of the mathematical structures of the crystal state in the manner that I outline next.

First I derive the constraints mentioned above:

(a) from $n\, S_{ab}\boldsymbol{l}_b = \nabla \wedge \boldsymbol{d}_a$ one has $\nabla \cdot (nS_{ab}\boldsymbol{l}_b) = 0$, $a = 1, 2, 3$, and manipulation gives

$$S_{ai}(\varepsilon_{ijk}S_{jk}) + \boldsymbol{l}_k \cdot \nabla S_{ak} = 0, \quad a = 1, 2, 3. \tag{5.2}$$

One might call (5.2) (a form of) the generalized Jacobi identity. In the case that S is constant, (5.2) reduces to (5.1);

(b) from $\nabla\nu = (\boldsymbol{l_a}\cdot\nabla\nu)\boldsymbol{d}_a$ one has $\nabla\wedge((\boldsymbol{l_a}\cdot\nabla\nu)\boldsymbol{d}_a) = \boldsymbol{0}$, and manipulation gives

$$S_{ab}F_a = \varepsilon_{bac}F'_aF_c, \quad a = 1, 2, 3, \tag{5.3}$$

where $F_a \equiv \boldsymbol{l_a}\cdot\nabla\nu$, $a = 1, 2, 3$, and $F'_a \equiv \frac{dF_a}{d\nu}$, $a = 1, 2, 3$.

Note that (5.2) is an algebraic condition on the points of C, whereas (5.3) is a set of ordinary differential equations to be satisfied along that curve. When S is constant, (5.3) is trivially satisfied.

Second, according to [17], [18], (5.2) and (5.3) together are sufficient for the local integrability of

$$nS_{ab}\boldsymbol{l}_b = \nabla\wedge\boldsymbol{d}_a, \quad \nabla\nu = F_a\boldsymbol{d}_a, \quad a = 1, 2, 3, \tag{5.4}$$

for the fields $\{\boldsymbol{l}_a(\cdot)\}$, given S, F_a as functions of ν. Therefore (5.2) and (5.3) are the only constraints on C, in general. But now I impose the extra condition mentioned in the introduction — I require that the third order nested Lie brackets be determined as linear combinations of the first $\{\boldsymbol{l}_a\}$ and second $\{\boldsymbol{L}_a\}$ order 'nested' Lie brackets. If this relation is known, then nested Lie brackets of all orders are determined as linear combinations of $\{\boldsymbol{l}_a\}, \{\boldsymbol{L}_a\}$, and so in Elzanowski and Preston's terminology [10] we have a lattice algebra of finite dimension.

Using (2.13), (2.19), and the Jacobi identity in the form $[\boldsymbol{l}_a, \boldsymbol{L}_a] = \boldsymbol{0}$, one finds that this assumption is equivalent to

$$S_{ai}(\varepsilon_{ijk}S_{jc}) + \boldsymbol{l}_k \cdot \nabla S_{ac} = f_{ack}(S), \quad a, c, k = 1, 2, 3, \tag{5.5}$$

where $f_{ack}(\cdot)$ is an affine function such that $f_{akk}(S) = 0$. Equation (5.5) implies that the quantities $\{F_a\}$ in (5.3) are quadratic in S (because by (4.2) one can choose indices a,c such that the second term in (5.5) is $\boldsymbol{l_k}\cdot\nabla\nu$, which is F_k), and it implies that (5.2) holds, in particular. Also (5.3) and (5.5) are algebraic conditions on (point values of) elastic invariants up to and including second order directional derivatives of S. Now one can progress without studying (5.3), (5.5) in detail, for according to [10], [9], there exists which a Lie group of transformations, of dimension > 3, (again denoted G) together with a group action $\lambda : G \times \mathbb{R}^3 \to \mathbb{R}^3$ such that the corresponding Lie algebra $\mathfrak{g}$ is homomorphic to the given lattice algebra. In other words, there is a Lie group G (of dimension greater that three) whose Lie algebra $\mathfrak{g}$ is such that the relation between the nested brackets of $\mathfrak{g}$ is the same as the relation between the nested Lie brackets of the vector fields discussed above.

This is an abstract structure defined (modulo isomorphism) from the 'concrete' lattice vector fields of the crystal state. It is the group action $\lambda : G \times \mathbb{R}^3 \to \mathbb{R}^3$ that ties the higher dimensional Lie group to the crystal state defined on $\Omega \subseteq \mathbb{R}^3$.

So the task to be addressed in section 7 is the following: how to connect a given crystal state with points of the classifying manifold satisfying (5.3), (5.5) *explicitly* with quantities defined on G. (This is entirely analogous to corresponding task in case (ii) above, where it turned out that the lattice vector fields were right invariant with respect to the corresponding group, modulo elastic deformation). I give some indications of how this is done in Section 7, for the moment I note only that the group action gives a projection from G to the lower dimensional manifold $\mathbb{R}^3$ (via $\lambda(\cdot, \mathbf{0}) : G \to \mathbb{R}^3$, say).

6. Discrete subgroups of three dimensional Lie groups

I confine attention, in this section, to crystal states where the material points $\boldsymbol{x} \in \Omega$ may be represented as elements of a three dimensional Lie group G with corresponding right invariant fields $\{\boldsymbol{l}_a(\cdot)\}$ satisfying (2.17) and $S =$ constant. The simplest case is when $S = 0$, then $\nabla \wedge \boldsymbol{d}_a = \boldsymbol{0}$, $a = 1, 2, 3$ and $\{\boldsymbol{d}_a(\cdot)\} = \{\nabla\tau_a(\cdot)\} = \{\tau_{a,i}(\cdot)\boldsymbol{e}_i\}$, say, for some independent 'potentials' $\{\tau_a(\cdot)\}$. Using $\boldsymbol{\tau}(\cdot)) \equiv (\tau_1(\cdot), \tau_2(\cdot), \tau_3(\cdot))$ as an elastic deformation, one transforms the crystal state to obtain lattice vector fields constant in Ω $(= \{\boldsymbol{e}_a\})$. It now follows from (2.17) that $\nabla_1\boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y}) =$ identity, so $\boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x} + \boldsymbol{f}(\boldsymbol{y})$ for some $\boldsymbol{f} : \mathbb{R}^3 \to \mathbb{R}^3$. Since $\boldsymbol{\chi}$ is a group composition function, $\boldsymbol{\chi}(\boldsymbol{0}, \boldsymbol{y}) = \boldsymbol{y}$, and we get finally that $\boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x} + \boldsymbol{y}$. So if $S = 0$ the group operation is addition of points (group elements) in $\mathbb{R}^3$, modulo the elastic deformation defined by the unknown potentials $\{\tau_a(\cdot)\}$. According to [16] the only discrete subgroups of $\mathbb{R}^3$, seen as an additive group, are the perfect lattices, so the study of symmetry of discrete structures associated with the continuum crystal state where $S = 0$ becomes traditional crystallography.

What is the role of the discrete subgroups of G in the case of constant $S \neq 0$, S satisfying (5.1)? It is envisaged at the outset that the integral lines of the lattice vector fields give information about the location of 'neighbouring' points/objects in some possibly discrete set that represents the microscopic/mesoscopic structure of the crystal, when one point/object is given. So, let us say that if there is a point of the structure at $\boldsymbol{x}(0) \in \mathbb{R}^3$, there are also points at $\boldsymbol{x}(1)$ and $\boldsymbol{x}(-1)$, where the curve $\{\boldsymbol{x} = \boldsymbol{x}(t); t \in \mathbb{R}\}$ is the integral curve of $\boldsymbol{l}_a(\cdot)$, $a = 1, 2, 3$:

$$\dot{\boldsymbol{x}}(t) \equiv \frac{d\boldsymbol{x}}{dt}(t) = \boldsymbol{l}_a(\boldsymbol{x}(t)), \quad a = 1, 2, 3. \tag{6.1}$$

Now it pays to introduce some notation, via (6.2), (6.3), $(6.4)_2$ below. Notice that because $\boldsymbol{l}_a(\cdot)$ is a right invariant field, it is determined by its value at $\boldsymbol{x} = \boldsymbol{0}$, by putting $\boldsymbol{x} = \boldsymbol{0}, \boldsymbol{\chi}(\boldsymbol{0}, \boldsymbol{y}) = \boldsymbol{y}$ in (2.17). Then if $\boldsymbol{p} \in \mathbb{R}^3, \boldsymbol{p} = p_i\boldsymbol{l}_i(\boldsymbol{0})$ say, and $\boldsymbol{p}(t)$ represents a point of the integral curve of the right invariant field $p_i\boldsymbol{l}_i(\boldsymbol{x})$, with arbitrary initial point $\boldsymbol{p}(0)$, one may define the mapping $\exp(t\boldsymbol{p}) : G \to G$ by

$$(\exp(t\boldsymbol{p}))\,(\boldsymbol{p}(0)) = \boldsymbol{p}(t), \quad \boldsymbol{p}(0) \in G \subseteq \mathbb{R}^3. \tag{6.2}$$

Also introduce the group element $e^{t\boldsymbol{p}}$ via

$$e^{t\boldsymbol{p}} \equiv (\exp(t\boldsymbol{p}))\,(\boldsymbol{0}). \tag{6.3}$$

It is an important fact that

$$(\exp(t\boldsymbol{p}))\,(\boldsymbol{x}) = \boldsymbol{\chi}(e^{t\boldsymbol{p}}, \boldsymbol{x}) \equiv e^{t\boldsymbol{p}}\boldsymbol{x}, \quad e^{t\boldsymbol{p}}, \boldsymbol{x} \in G, \tag{6.4}$$

where the juxtaposition of group elements, as in $(6.4)_2$, is to represent group multiplication. In other words, the process of exponentiation, defined via the right invariant fields $\{\boldsymbol{l}_a(\cdot)\}$ maps an element $\boldsymbol{p}$ of the Lie algebra to the group G. Note that the bracket operation in the algebra can be defined in a familiar way.

So one envisages that, when we are dealing with right invariant fields in a Lie group G, that if there is a point of some representative structure at $\mathbf{0}$, then there are also points at $e^{\boldsymbol{l}_a}$, and by iterating also at $e^{\boldsymbol{l}_b}e^{\boldsymbol{l}_a}$, etc.. So the relevant set of points is a subgroup of G.

Now the "crystallographic restriction" which produces the perfect lattices of crystallography is the requirement that iteration of certain symmetry operations produces a *discrete* set of points (i.e. a set of points with nonzero minimum pairwise separation). We adopt the analogous requirement here, that the set of subgroup elements (as points of $\mathbb{R}^3$) be discrete. This restriction is a strong requirement, [19], [20], which restricts the value of S, the composition function $\boldsymbol{\chi}$ and the form of the Lie algebra $\mathfrak{g}$. In fact there are just three classes of three dimensional Lie groups that have discrete subgroups, according to [19], and I concentrate here on results available for just one of those classes. So take

$$\boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{y}) \equiv \boldsymbol{x} + \boldsymbol{y} + \tfrac{1}{2}\mu\boldsymbol{p}(\boldsymbol{p}\cdot\boldsymbol{x}\wedge\boldsymbol{y}), \tag{6.5}$$

where it turns out that μ must be a rational number, and that the components of $\boldsymbol{p} \in \mathbb{R}^3$ can be taken to be relatively prime integers, if there are to exist discrete subgroups $D \subset G$. One calculates that, with $\boldsymbol{e}_a \equiv \boldsymbol{l}_a(\mathbf{0})$,

$$\boldsymbol{l}_a(\boldsymbol{x}) = \boldsymbol{e}_a + \tfrac{1}{2}\mu\boldsymbol{p}(\boldsymbol{x}\wedge\boldsymbol{p}\cdot\boldsymbol{e}_a), \quad e^{\boldsymbol{x}} = \boldsymbol{x}, \quad a = 1, 2, 3, \tag{6.6}$$

by the process give above, so that from $(6.6)_2$ elements of the Lie algebra can be identified with elements of the group. The structure constants are $C_{ijk} = \mu\varepsilon_{rjk}p_ip_r$ and so

$$[\boldsymbol{x}, \boldsymbol{y}] = \mu\boldsymbol{p}(\boldsymbol{p}\cdot\boldsymbol{x}\wedge\boldsymbol{y}). \tag{6.7}$$

Define the commutator of group elements $(\boldsymbol{x}, \boldsymbol{y}) \equiv \boldsymbol{x}^{-1}\boldsymbol{y}^{-1}\boldsymbol{x}\boldsymbol{y}$, where the inverse group element $\boldsymbol{x}^{-1}$ is such that $\boldsymbol{\chi}(\boldsymbol{x}^{-1}, \boldsymbol{x}) = \boldsymbol{\chi}(\boldsymbol{x}, \boldsymbol{x}^{-1}) = \mathbf{0}$, so $\boldsymbol{x}^{-1} = -\boldsymbol{x}$ in this case. One finds that

$$(\boldsymbol{x}, \boldsymbol{y}) = [\boldsymbol{x}, \boldsymbol{y}]. \tag{6.8}$$

The commutator is a 'finite' version of the Burgers vectors (or Lie bracket, more precisely) — $(\boldsymbol{x}, \boldsymbol{y})$ is the point reached by flow along the integral curve defined by $\boldsymbol{y}$, followed by that defined by $\boldsymbol{x}$, and so on.

Now let D be any discrete subgroup of G. According to [21], one can choose a set of generators of D, $\{\boldsymbol{c}_1, \boldsymbol{c}_2, \boldsymbol{c}_3\}$, such that

$$\boldsymbol{c}_3 = \vartheta \boldsymbol{p} \text{ for some } \vartheta \in \mathbb{R}, \quad (\boldsymbol{c}_1, \boldsymbol{c}_2) = \boldsymbol{c}_3^k, \text{ for some } k \in \mathbb{Z}. \tag{6.9}$$

If follows that

$$(\boldsymbol{c}_1, \boldsymbol{c}_3) = (\boldsymbol{c}_2, \boldsymbol{c}_3) = \boldsymbol{0}. \tag{6.10}$$

One can use these relations to show that any group element has the form

$$\boldsymbol{c}_1^\alpha \boldsymbol{c}_2^\beta \boldsymbol{c}_3^\gamma, \quad \alpha, \beta, \gamma \in \mathbb{Z}. \tag{6.11}$$

(G is not a commutative group, so (6.11) is a non-trivial fact. Recall, for purposes of comparison, that an arbitrary point in a perfect lattice with basis $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ has the form $\alpha \boldsymbol{e}_1 + \beta \boldsymbol{e}_2 + \gamma \boldsymbol{e}_3$, $\alpha, \beta, \gamma \in \mathbb{Z}$.)

So, in physical terms, this group corresponds to a uniformly distributed system of screw dislocations with Burgers vector $k\boldsymbol{c}_3$ (since successive flows along $\boldsymbol{c}_2, \boldsymbol{c}_1, \boldsymbol{c}_2^{-1}, \boldsymbol{c}_1^{-1}$ lead to $\boldsymbol{c}_3^k = k\boldsymbol{c}_3$). Note that the integer k can be determined in terms of μ and $\boldsymbol{p}$, see [22].

In crystallography, the set of changes of basis of a perfect lattice can be regarded as a symmetry group (related to the cubic, tetragonal, etc, crystal classes) — in the case at hand, the different choice of generators of D play a similar role, see [23, 24]. For the nilpotent group G defined by (6.5) one has also:

Theorem 6.1. [21] *Let D be a discrete subgroup of G. Then every automorphism of D can be uniquely extended to an automorphism of G.*

Remark 6.1. *The automorphisms of D are bijections of the set of corresponding group elements which preserve the group multiplication. The result says that any such bijection can be extended to a smooth bijection of the elements of the ambient group G, preserving group multiplication. It is an assertion that D is 'rigid' in G, that the symmetries of the points of D determine symmetries of the continuum. In my view this is a fundamental result which gives a rigorous connection between discrete and continuous models of the crystal state.*

7. Discrete subgroups of higher dimensional Lie groups

In the case that $S =$ constant, the lattice vector fields can be interpreted as right invariant fields on a Lie group. We seek an analogous interpretation in the case that $\nabla S \neq 0$, where the classifying manifold is subject to the constraints (5.3), (5.5), and there exists a Lie group of dimension strictly greater than the number of lattice vector fields with Lie algebra homomorphic to the given lattice algebra. I simplify, in this section, by assuming that the crystal state consists of two lattice vector fields defined in $\Omega \subset \mathbb{R}^2$, since the emphasis in this paper is on ideas rather than detailed calculation. I also show how to obtain discrete structures (not necessarily discrete subgroups of Lie groups) in $\mathbb{R}^2$ which derive from the crystal state.

To fix ideas, I choose two specific lattice vector fields in Ω, with Ω such that $(x_1, x_2) \in \Omega$ implies $x_1 > 0$, to keep the calculations simple. So let

$$\boldsymbol{l}_1(x_1, x_2) = (1, 0),\ \boldsymbol{l}_2(x_1, x_2) = (0, -x_1). \tag{7.1}$$

Calculate and define

$$[\boldsymbol{l}_1, \boldsymbol{l}_2] = (0, 1) \equiv \boldsymbol{l}_3. \tag{7.2}$$

Note that $[\boldsymbol{l}_1, \boldsymbol{l}_2]$ cannot be expressed in terms of a constant coefficient combination of $\boldsymbol{l}_1, \boldsymbol{l}_2$. and that $[\boldsymbol{l}_a, [\boldsymbol{l}_b, \boldsymbol{l}_c]] = \boldsymbol{0}$, $a, b, c = 1, 2$. So we have a three dimensional nilpotent lattice algebra. Let $\tilde{G}$ be a three dimensional Lie group with composition $\tilde{\boldsymbol{\chi}}$ given by (with $\boldsymbol{g} \equiv (a, 1, m), \bar{\boldsymbol{g}} \equiv (\bar{a}, \bar{1}, \bar{m})$ elements of $\tilde{G}$):

$$\tilde{\boldsymbol{\chi}}(\boldsymbol{g}, \bar{\boldsymbol{g}}) = (a + \bar{a}, l + \bar{l}, m + \bar{m} + l\bar{a}). \tag{7.3}$$

The group acts on $\mathbb{R}^2$ via the group action $\lambda : \tilde{G} \times \mathbb{R}^2 \to \mathbb{R}^2$ defined by

$$\lambda(\boldsymbol{g}, \boldsymbol{x}) = (x_1 + a,\ x_2 - l(x_1 + a) + m), \tag{7.4}$$

and one can check that

$$\lambda(\boldsymbol{g}, \lambda(\bar{\boldsymbol{g}}, \boldsymbol{x})) = \lambda(\tilde{\boldsymbol{\chi}}(\boldsymbol{g}, \bar{\boldsymbol{g}}), \boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^2. \tag{7.5}$$

The right invariant fields $\nabla_1 \tilde{\boldsymbol{\chi}}(\boldsymbol{0}, \boldsymbol{g}) \boldsymbol{e}_a$ on $\tilde{G}$ are

$$\tilde{\boldsymbol{l}}_1 = (1, 0, l), \tilde{\boldsymbol{l}}_2 = (0, 1, 0), \tilde{\boldsymbol{l}}_3 = (0, 0, 1). \tag{7.6}$$

One calculates that $[\tilde{\boldsymbol{l}}_1, \tilde{\boldsymbol{l}}_2] = \tilde{\boldsymbol{l}}_3$, and that the other Lie brackets are zero. So $\tilde{\mathfrak{g}}$, the Lie algebra of $\tilde{G}$, is homomorphic to the given lattice algebra, confirming the existence of a Lie group with this property as asserted in [9].

Now let $\nabla_1 \lambda = (\lambda_{\alpha,j}), \alpha = 1, 2, j = 1, 2, 3$, denote the gradient of λ with respect to its first argument, and similarly for $\nabla_1 \tilde{\boldsymbol{\chi}} = (\tilde{\chi}_{j,k})$, $j, k = 1, 2, 3$. Differentiating (7.5) with respect to $\boldsymbol{g}$, putting $\boldsymbol{g} = \boldsymbol{0}, \boldsymbol{x} = \boldsymbol{0}$, using $\tilde{\boldsymbol{\chi}}(\boldsymbol{0}, \bar{\boldsymbol{g}}) = \bar{\boldsymbol{g}}$ and finally replacing $\bar{\boldsymbol{g}}$ by $\boldsymbol{g}$ one obtains:

$$\lambda_{\alpha,j}(\boldsymbol{g},\mathbf{0})\tilde{\chi}_{j,k}(\mathbf{0},\boldsymbol{g}) = \lambda_{\alpha,k}\left(\mathbf{0},\lambda(\boldsymbol{g},\mathbf{0})\right). \tag{7.7}$$

Now the right invariant fields on $\tilde{G}$ are $\nabla_1\tilde{\boldsymbol{\chi}}(\mathbf{0},\boldsymbol{g})\boldsymbol{e}_a = (\tilde{\chi}_{i,a})$. Define three fields $\left\{\bar{\boldsymbol{l}}_a(\cdot)\right\}$ on $\mathbb{R}^2$ by $\bar{\boldsymbol{l}}_a(\boldsymbol{x}) = (\lambda_{\alpha,a}(\mathbf{0},\boldsymbol{x})), a = 1,2,3, \boldsymbol{x} \in \mathbb{R}^2$. Then (7.7) reads

$$\nabla\boldsymbol{u}(\boldsymbol{g})\tilde{\boldsymbol{l}}_a(\boldsymbol{g}) = \bar{\boldsymbol{l}}_a(\boldsymbol{u}(\boldsymbol{g})), \quad \boldsymbol{g} \in G, \tag{7.8}$$

if we define the 'projection' $\boldsymbol{u} : \tilde{G} \to \mathbb{R}^2$ by

$$\boldsymbol{u}(\boldsymbol{g}) = \lambda(\boldsymbol{g},\mathbf{0}). \tag{7.9}$$

The fields $\left\{\bar{\boldsymbol{l}}_a(\cdot)\right\}$ are push-forwards to $\mathbb{R}^2$ of the right invariant fields on the group — one might also say the right invariant fields are transformed by the 'singular elastic deformation' $\boldsymbol{u} : \tilde{G} \to \mathbb{R}^2$ to the fields $\left\{\bar{\boldsymbol{l}}_a(\cdot)\right\}$. One calculates that

$$\bar{\boldsymbol{l}}_a(\boldsymbol{x}) \equiv \boldsymbol{l}_a(\boldsymbol{x}), \quad a = 1,2,3, \boldsymbol{x} \in \Omega. \tag{7.10}$$

Thus one can interpret the given lattice vector fields, in Ω, as fields obtained by 'singular' elastic deformation of the right invariant fields on $\tilde{G}$. (The result is a little artificial — in general one would need a further local elastic deformation in order to recover the original fields). Also, note that the fields $\left\{\bar{\boldsymbol{l}}_a(\cdot)\right\}$ are defined on $\mathbb{R}^2$, a priori, so that an appropriate restriction of these fields is implicit in (7.10).

Finally, in this section, the simplest way to construct a possibly discrete set of points in $\mathbb{R}^2$ which represents the higher dimensional Lie group structure of the crystal state seems to be the following: let $\tilde{D}$ be a discrete subgroup of the higher dimensional group $\tilde{G}$ and project D to $\mathbb{R}^2$ via the singular elastic deformation $\boldsymbol{u} : \tilde{G} \to \mathbb{R}^2$. This gives

$$\lambda(\tilde{D},\mathbf{0}), \tag{7.11}$$

which is the orbit of $\mathbf{0} \in \mathbb{R}^2$ with respect to the group action, restricted to $\tilde{D}$. In the particular example above we can use information about the discrete subgroups D of the group G with composition function (6.5), in section 6: let $\boldsymbol{\kappa} : \mathbb{R}^3 \to \mathbb{R}^3$ be the mapping

$$\boldsymbol{\kappa}(a,l,m) = (a,l,m - \tfrac{1}{2}al),\ \boldsymbol{\kappa}^{-1}(p,q,r) = (p,q,r + \tfrac{1}{2}pq). \tag{7.12}$$

This mapping changes the composition function $\tilde{\boldsymbol{\chi}}$ to the composition function (6.5) with $\mu = 1$, $\boldsymbol{p} = \boldsymbol{e}_3$, and the corresponding group has discrete subgroups by the remark that follows (6.5). Cermelli and Parry, in[22], found the discrete subgroups D with generators $\{e^{\boldsymbol{e}_a}\}$ for this composition function (6.5). Working through the details, it turns out that

$$\tilde{D} = \boldsymbol{\kappa}^{-1}(D) = \mathbb{Z}^3,\ \lambda(\tilde{D}, \mathbf{0}) = \mathbb{Z}^2, \tag{7.13}$$

so that in this case the 'representative' set of points in $\mathbb{R}^2$ has a lattice structure. The corresponding points in Ω are $\mathbb{Z}^2 \cap \Omega$. It appears that this lattice structure is not to be expected in general, though. Indeed, one aim of the work is to set out a constitutive framework more general than that which leads to the perfect crystallographic structures — one would hope to include the quasicrystals, for example, and the projections that appear above are certainly reminiscent of some techniques in that area. Also, even if there is no evident group structure in sets of points produced as above, one can find 'continuum mechanical type' symmetries by calculating which different choices of values of the constitutive variables produce the same representative set of points.

8. Summary and future work

The purpose of this paper has been two-fold,

(i) to provide a means of quantifying inelastic behaviour in Davini's continuum model of defective crystals, by constructing bases of invariant integrals and elastic invariants;

(ii) to illustrate the construction of discrete structures naturally associated with such continua in some non-trivial cases.

The study was facilitated by two assumptions:

(iii) the crystal states under consideration allow neutral deformations, i.e. partial differential equations (4.1) have non-unique solutions for $\{\boldsymbol{l}'_a(\cdot)\}$ given $\{\boldsymbol{l}_a(\cdot)\}$. This non-uniqueness can be characterized in terms of the rearrangement of vector fields, or the 'slip mechanism' of plasticity theory – so slip is given a place in the mathematical formulation which is subordinate to the construction of the invariants, and this is strong motivation for this assumption;

(iv) given three lattice vector fields one may calculate the corresponding Lie brackets (or equivalently, the Burgers vector fields), and one may iterate this procedure, so constructing nested Lie brackets of any order. The second assumption is that this procedure produces a finite dimensional Lie algebra of vector fields, called the 'lattice algebra' by Elżanowski and Preston. There is then a corresponding Lie group, generally of a finite dimension greater than the number of lattice vector fields. This is a pragmatic assumption, made in order to understand what kind of mathematical structures relate to continua with non-constant dislocation density.

The discussion focussed on the following items:

(v) the role of the classifying manifold as an all inclusive list of plastic strain variables (elastic invariants). Since crystal states with the same classifying manifold C are locally elastically related (in the sense that, given points $\boldsymbol{x}_0 \in \Omega, \boldsymbol{x}'_0 \in \Omega'$ which correspond to the same point on the classifying manifold, there are neighbourhoods of $\boldsymbol{x}_0, \boldsymbol{x}'_0$ such that lattice vector fields $\{\boldsymbol{l}_a(\cdot)\}, \{\boldsymbol{l}'_a(\cdot)\}$ defined on those neighbourhoods are elastically related), it follows that
   (a) crystal states where C is a single point have the self-similarity (2.17), loosely,
   (b) neutrally related states are locally elastically related;

(vi) the constraints (5.2), (5.3) which apply to the classifying manifold (and the third constraint (5.5) which applies if one adopts assumption (iv)).

According to [17, 18] if the first two constraints on C hold, then there is a set of lattice vector fields $\{\boldsymbol{l}_a(\cdot)\}$ satisfying (5.4), locally, i.e. no other constraints are necessary for that purpose;

(vii) the intimate connection between the continuum theory of defects and the theory of Lie groups. In the case that the Lie group has dimension 3, canonical forms of corresponding discrete subgroups are known, and symmetries of these groups have been calculated in [23, 24]. In the case of a particular group of dimension greater than the number of lattice vector fields, one way to find corresponding discrete structures is given in section 7.

Short term objectives following on from this work include the following:

(viii) since the classifying manifold, subject to (5.2), (5.3), quantifies all continuous distributions of defects modulo local elastic deformation, one might attempt to catalogue the lattice vector fields which solve (5.5), modulo local elastic deformation. The task is more tractable if one makes the additional assumption (iv), for then the general constraints are simplified and the general theory of low-dimensional homogeneous spaces becomes relevant, e.g. [25];

(ix) it becomes apparent that there are other quite natural ways to construct discrete structures associated with fields with non-constant dislocation density, if one considers the constraints in detail (i.e., the method employed in section 7 is not the only one). It will be an important task to consider the symmetries of these structures (noting that there is no associated group structure, in general);

(x) it should be possible to interpret the neutral deformations at the discrete level and so judge whether or not those changes of state are dissipative, e.g., by examining the consequences of the assumption that they are not dissipative, as Fonseca and Parry did for perfect crystals in [26].

In brief, this particular systematic approach to the geometry of defects includes many well-known useful concepts and introduces others less well-known by connecting to different mathematical areas. Also it leads to the prospect of a catalogue of quite general low-dimensional defective crystal structures, continuous and discrete, with all the modelling and material design possibilities that the existence of such a catalogue entails.

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