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Material Symmetry in Slightly Defective Crystals

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1. INTRODUCTION

I outline ideas which are relevant to the theory of continuous distributions of defects in solid crystals, and also to the relation of that theory with the view that a crystal is composed of a collection of atoms with some kind of translational order.

There are two images that come to mind when one thinks of a solid crystal. Firstly, there is the idea that a crystal is composed of atoms which arrange themselves in relatively stable positions at, or close to, the sites of a regular lattice in $\mathbb{R}^3$. Then, slight modifications of this picture are fairly easy to visualise; for instance, one may suppose that a 'half-plane of atoms' is inserted (from infinity) between appropriate lattice planes, and imagine that the structure of the crystal is modified only in the vicinity of this half-plane, to accommodate the introduction of these atoms. This is the 'discrete' picture of an edge dislocation, and it is traditional to assert that the number of singular lines (defined by defects of this, or similar, type) which cross a typical square centimetre section of metal crystal is of the order of 10^6. Also, there is a very inventive literature which documents methods by which such defects may interact, usually based on lattice geometry arguments. Moreover, many theories of plastic deformation take their inspiration from the slip mechanism, whereby lattice planes (of atoms) translate relative to adjacent planes of the same family. More specifically, some such theories postulate that the plastic strain rate can always be represented as the superposition of a finite number of such slips on specific lattice planes. Thus the discrete structure allows for a plethora of geometric deformation processes and associated mechanical theories, but none of these theories accounts satisfactorily for the description or evolution of the intricate and dense network of defects that typically infests a solid crystal.

Secondly, there are the geometric theories of smooth vector fields defined on a region $\Omega \subset \mathbb{R}^3$. These vector fields are imagined to characterise the crystal structure in some way which is not made precise. For instance, they may be thought of as interpolating the position vectors of nearest neighbours of atoms, though then one would imagine that such interpolations would be highly oscillatory, or not smooth. On the other hand, they may perhaps be obtained from such fields by an inexplicit smoothing or averaging procedure. In any case, there is an act of faith involved in stating that it is sufficient to consider smooth vector fields in this context. However, with this faith, one has available the beautiful apparatus of differential geometry and then it is an issue, whether or not one can recover analogues of the geometric mechanisms which provide the richness of the discrete theories, with this approach.

The inspirational work of Kondo[6], Kröner [7],[8], Bilby [2] and others in the 1950's provides an identification of Cartan's torsion with the dislocation density tensor of phenomenological theories, but it does not provide the analogue of slip (for example). Here I outline a geometric framework where the slips appear as particular kinds of rearrangements of vector fields, and briefly describe a naive attempt to connect discrete and smooth theories.

2. Davini's Model of a Crystal

In 1986, Davini [3] suggested that the central, primitive quantities in a continuum theory of the mechanics of solid crystals should be taken as

i. three linearly independent lattice vector fields $\boldsymbol{d}_1(\cdot)$, $\boldsymbol{d}_2(\cdot)$, $\boldsymbol{d}_3(\cdot)$,

ii. a mass density field $\rho(\cdot)$,

each of these fields defined over a region Ω (identified as the current placement of the continuum that makes up the crystal), and each of these fields varying smoothly (say, analytically) over Ω. In [4], Davini and I introduced a corresponding notion of *crystal state*, Σ, defined by these four fields;

$$\Sigma = \{(\boldsymbol{d}_a(\cdot), \rho(\cdot), \Omega)\,; \quad a = 1,\ 2,\ 3\}\,, \tag{1}$$

and addressed what seemed, to us, to be a fundamental issue in the theories of elasticity and plasticity: "If two crystal states are given, then are they elastically related to one another or not?". Here, we take crystal states Σ and

$$\Sigma^* \equiv \{(\boldsymbol{d}^*_a(\cdot), \rho^*(\cdot), \Omega^*)\,; \quad a = 1, 2, 3\}\,, \tag{2}$$

to be elastically related to one another if and only if there exists a diffeomorphism $\boldsymbol{u} : \Omega \to \Omega^* = \boldsymbol{u}(\Omega)$ such that

$$\begin{aligned} \boldsymbol{d}_a^* (\boldsymbol{u}(\boldsymbol{x})) &= \nabla \boldsymbol{u}(\boldsymbol{x}) \boldsymbol{d}_a(\boldsymbol{x}), \quad a = 1,\ 2,\ 3; \\ \rho^* (\boldsymbol{u}(\boldsymbol{x})) &= [\det \nabla \boldsymbol{u}(\boldsymbol{x})]^{-1} \rho(\boldsymbol{x}), \boldsymbol{x} \in \Omega. \end{aligned} \tag{3}$$

To restate the issue, how does one decide if there exists a diffeomorphism $\boldsymbol{u}$ such that (3) holds if the fields $\boldsymbol{d}_a(\cdot)$, $\boldsymbol{d}_a^*(\cdot)$, $\rho(\cdot)$, $\rho^*(\cdot)$, $a = 1,\ 2,\ 3$, are given over prescribed domains Ω and Ω^*? To proceed, let us introduce the *dual lattice vector fields* $\boldsymbol{d}^1(\cdot)$, $\boldsymbol{d}^2(\cdot)$, $\boldsymbol{d}^3(\cdot)$ which have the property that

$$\boldsymbol{d}^a(\boldsymbol{x}) \cdot \boldsymbol{d}_b(\boldsymbol{x}) = \delta_b^a\ , \quad a,\ b = 1,\ 2,\ 3, \quad \boldsymbol{x} \in \Omega, \tag{4}$$

define

$$\begin{aligned} n(\boldsymbol{x}) &\equiv \det \{\boldsymbol{d}^a(\boldsymbol{x})\} \equiv \boldsymbol{d}^1(\boldsymbol{x}) \cdot \boldsymbol{d}^2(\boldsymbol{x}) \wedge \boldsymbol{d}^3(\boldsymbol{x}), \\ S^{ab}(\boldsymbol{x}) &= \boldsymbol{d}^a(\boldsymbol{x}) \cdot \nabla \wedge \boldsymbol{d}^b(\boldsymbol{x}), \end{aligned} \tag{5}$$

and abbreviate the notation introduced in (1) above by writing loosely

$$\Sigma = \{\boldsymbol{d}_a,\ \rho,\ \Omega\}\,. \tag{6}$$

Then if we notice that (3) implies

$$\begin{aligned} \boldsymbol{d}^{a*} (\boldsymbol{u}(\boldsymbol{x})) &= [\nabla \boldsymbol{u}(\boldsymbol{x})]^{-T} \boldsymbol{d}^a(\boldsymbol{x}), \\ (\nabla \wedge \boldsymbol{d}^{a*}) (\boldsymbol{u}(\boldsymbol{x})) &= [\det \nabla \boldsymbol{u}(\boldsymbol{x})]^{-1} \nabla \boldsymbol{u}(\boldsymbol{x}) \nabla \wedge \boldsymbol{d}^a(x), \\ n^* (\boldsymbol{u}(\boldsymbol{x})) &= [\det \nabla \boldsymbol{u}(\boldsymbol{x})]^{-1} n(x), \end{aligned} \tag{7}$$

it follows from (5) and (7) that

$$\frac{S^{ab*} (\boldsymbol{u}(\boldsymbol{x}))}{n^* (\boldsymbol{u}(\boldsymbol{x}))} = \frac{S^{ab}(\boldsymbol{x})}{n(\boldsymbol{x})}\ , \quad x \in \Omega. \tag{8}$$

Equations (7) and (8) are necessarily true, if (3) holds, and one can list infinitely many more such necessary conditions that Σ and Σ^* are elastically related to one another. (See [4], [5] for explicit details).

Now, it is productive to notice, from (8), that

$$\underset{\boldsymbol{y} \in \Omega^*}{\text{Range}} \ \frac{S^{ab*}(\boldsymbol{y})}{n^*(\boldsymbol{y})} = \underset{\boldsymbol{x} \in \Omega}{\text{Range}} \ \frac{S^{ab}(\boldsymbol{x})}{n(\boldsymbol{x})}, \tag{9}$$

and that, crucially, the left hand side of (9) can be calculated from knowledge of the state Σ^*, the right hand side of (9) can be calculated if one knows Σ.

(Note that $\boldsymbol{y} \equiv \boldsymbol{u}(\boldsymbol{x})$ ranges over $\Omega^* \equiv \boldsymbol{u}(\Omega)$ as $\boldsymbol{x}$ ranges over Ω, since $\boldsymbol{u}$ is diffeomorphism). The manifold

$$\left\{ \left(\frac{S^{ab}(\boldsymbol{x})}{n(\boldsymbol{x})} \right); a, b = 1,\ 2,\ 3,\quad x \in \Omega \right\}, \tag{10}$$

is thus an *elastic invariant* of the crystal state Σ in the sense that (9) holds if (3) holds. In fact, it should now be clear that if one constructs a *scalar* field $\mu_\Sigma(\cdot)$ from the primitive field quantities $\boldsymbol{d}_a(\cdot)$, $\rho(\cdot)$ and their derivatives of any order, so that

$$\mu_\Sigma(\boldsymbol{x}) = \mu\left(\boldsymbol{x},\ \boldsymbol{d}_a(\boldsymbol{x}),\ \nabla \boldsymbol{d}_a(\boldsymbol{x}),\ \nabla^2 \boldsymbol{d}_a(\boldsymbol{x}),\ \ldots,\ \rho(\boldsymbol{x}),\ \nabla\rho(\boldsymbol{x}),\ \nabla^2\rho(\boldsymbol{x}),\ \ldots\right). \tag{11}$$

where μ is a given real valued function, and $\mu_\Sigma(\cdot)$ is such that

$$\mu_{\Sigma^*}\left(\boldsymbol{u}(\boldsymbol{x})\right) = \mu_\Sigma(\boldsymbol{x}), \tag{12}$$

when (3) holds, then

$$\underset{\boldsymbol{y} \in \Omega^*}{\text{Range}}\ \mu_{\Sigma^*}(\boldsymbol{y}) = \underset{\boldsymbol{x} \in \Omega}{\text{Range}}\ \mu_\Sigma(\boldsymbol{x}) \tag{13}$$

and the manifold $\{(\mu_\Sigma(\boldsymbol{x}))\,;\ \boldsymbol{x} \in \Omega\}$ is an elastic invariant of the crystal state Σ. Note that I show in [11], see also [4], that there is an infinite number of different choices of scalar fields $\mu_\Sigma(\cdot)$.

3. Cartan's Classifying Manifold

Define the fundamental set $\mathcal{F}$ of scalar invariants of the crystal state Σ as the set of fields

$$\left\{1,\ \frac{S^{ab}}{n}(\cdot),\ (\boldsymbol{d}_c \cdot \nabla)\frac{S^{ab}}{n}(\cdot), \frac{\rho}{n}(\cdot),\ (\boldsymbol{d}_c \cdot \nabla)(\frac{\rho}{n})(\cdot); a,\ b,\ c = 1,\ 2,\ 3. \right\} \tag{14}$$

I refer the reader to [12] and to Arnold [1] for a discussion of topological properties of integrals associated with some of these fields. From this fundamental set $\mathcal{F}$ define Cartan's *classifying manifold* T as

$$T = \{\nu(\boldsymbol{x}),\ (\boldsymbol{d}_a \cdot \nabla)\nu(\boldsymbol{x}), (\boldsymbol{d}_b \cdot \nabla)(\boldsymbol{d}_a \cdot \nabla)\nu(\boldsymbol{x}); a,\ b = 1,\ 2,\ 3,\ \nu \in \mathcal{F},\ \boldsymbol{x} \in \Omega\} \tag{15}$$

This is (at most) a three dimensional manifold in $R^{(1+3^2+3^3+1+3)(1+3+3^2)}$, and one can check that it is an elastic invariant of Σ by verifying that $(\boldsymbol{d}_a \cdot \nabla)\nu(\cdot)$ is a scalar if $\nu(\cdot)$ is a scalar. Later in the work, I shall employ the following result of Cartan, taken from lecture notes of Olver[9], given here in a form which is appropriate to this context.

THEOREM 1. *Let Σ, Σ^* (c.f. definitions (1), (2)) have classifying manifolds T, T^*. Suppose that T and T^* overlap, in the sense that*

$$\mu_\Sigma(\boldsymbol{x}_0) = \mu_{\Sigma^*}(\boldsymbol{x}_0^*),$$

for some $(\boldsymbol{x}_0, \boldsymbol{x}_0^*) \in \Omega \times \Omega^*$, and for all

$$\mu_\Sigma(\cdot) \in \{\nu(\cdot),\ (\boldsymbol{d}_a \cdot \nabla)\nu(\cdot),\ (\boldsymbol{d}_b \cdot \nabla)(\boldsymbol{d}_a \cdot \nabla)\nu(\cdot); a, b = 1,\ 2,\ 3,\ \nu \in \mathcal{F}\}.$$

Then for any such $(\boldsymbol{x}_0,\ \boldsymbol{x}_0^*)$, there exists a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_0}$ defined on a neighbourhood $N_{\boldsymbol{x}_0}$ of $\boldsymbol{x}_0$ in Ω such that

$$\boldsymbol{d}_a^*\,(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})) = \nabla \boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})\boldsymbol{d}_a(\boldsymbol{x}),\ \boldsymbol{x} \in N_{\boldsymbol{x}_0},$$

and

$$\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x}_0) = \boldsymbol{x}_0^*.$$

NOTES

1. For the purposes of this theorem, the hypotheses regarding the field $\rho(\cdot)$ are spurious.
2. The theorem provides sufficient conditions that Σ, Σ^* are such that $(3)_1$ holds *locally*, and we shall be vitally concerned in the sequel with the mechanism that obstructs a global definition of the field $\boldsymbol{u}(\cdot)$ in $(3)_1$.

4. NEUTRAL DEFORMATIONS

There are other objects, apart from the scalars considered above, which provide natural elastic invariants of Σ. For example, there are the 'Burger's numbers' $\oint_\zeta \boldsymbol{d}^a(\boldsymbol{x}) \cdot \boldsymbol{dx}$, where ζ is any closed circuit in Ω - it is an easy calculation to show that

$$\oint_{\zeta^* \equiv \boldsymbol{u}(\zeta)} \boldsymbol{d}^{a*}(\boldsymbol{y}) \cdot \boldsymbol{dy} = \oint_\zeta \boldsymbol{d}^a(\boldsymbol{x}) \cdot \boldsymbol{dx}, \tag{16}$$

when $(3)_1$, and hence $(7)_1$, hold. In the same way, one finds that

$$\oint_\zeta \nu(\boldsymbol{x})\boldsymbol{d}^a(\boldsymbol{x})\cdot d\boldsymbol{x},\ \int_V \nu(\boldsymbol{x})n(\boldsymbol{x})dV_{\boldsymbol{x}},\ \nu\in\mathcal{F},\ V\subset\Omega, \tag{17}$$

are elastic invariants, in the obvious sense. Also, one could construct an infinite number of other, different, invariants of each of the two types given in (17). Now ask the following question; if the *finite* list of elastic invariants of type (17) match in Σ, Σ^*, in the sense that there exists a diffeomorphism $\boldsymbol{\theta} = \Omega \to \boldsymbol{\theta}(\Omega) \equiv \Omega^*$ such that

$$\oint_\zeta \nu(\boldsymbol{x})\boldsymbol{d}^a(\boldsymbol{x})\cdot d\boldsymbol{x} = \oint_{\boldsymbol{\theta}(\zeta)} \nu^*(\boldsymbol{\theta}(\boldsymbol{x}))\boldsymbol{d}^{a*}(\boldsymbol{x})\cdot d\boldsymbol{\theta}(\boldsymbol{x}),\ \text{etc.},\ \nu\in\mathcal{F}, \tag{18}$$

are the two states Σ, Σ^* elastically related to one another, in the sense that (3) holds ? Davini and I show in [4] that if the invariants (18) match, then all (the infinite number of) such invariants match. Moreover let $\Sigma' = \{\boldsymbol{d}'_a,\ \rho',\ \Omega\}$ be defined as the 'elastic pre-image' or 'pull-back' of Σ^*, so that

$$\begin{aligned} \boldsymbol{d}'_a\left(\boldsymbol{\theta}^{-1}(\boldsymbol{y})\right) &= (\nabla\boldsymbol{\theta}^{-1})(\boldsymbol{y})\boldsymbol{d}^*_a(\boldsymbol{y}), \\ \rho'\left(\boldsymbol{\theta}^{-1}(\boldsymbol{y})\right) &= \left[\det(\nabla\boldsymbol{\theta}^{-1})(\boldsymbol{y})\right]^{-1}\rho(\boldsymbol{y}), \quad y\in\boldsymbol{\theta}(\Omega)\equiv\Omega^*. \end{aligned} \tag{19}$$

Then (18) holds if and only if

$$\oint_\zeta \nu(\boldsymbol{x})\boldsymbol{d}^a(\boldsymbol{x})\cdot d\boldsymbol{x} = \oint_\zeta \nu'(\boldsymbol{x})\boldsymbol{d}^{a\prime}(\boldsymbol{x})\cdot d\boldsymbol{x},\quad \text{etc.},\ \nu\in\mathcal{F}, \tag{20}$$

and it follows, since ζ and V are arbitrary, that

$$[\nabla\wedge(\nu\boldsymbol{d}^a)](\boldsymbol{x}) = [\nabla\wedge(\nu'\boldsymbol{d}^{a\prime})](\boldsymbol{x}),\ (\nu'n')(\boldsymbol{x}) = (\nu n)(\boldsymbol{x}),\ \nu\in\mathcal{F},\ x\in\Omega. \tag{21}$$

One deduces from this last set of equations, (21), by taking $\nu\equiv 1$ to begin with, that

$$\nabla\wedge\boldsymbol{d}^{a\prime} = \nabla\wedge\boldsymbol{d}^a,\ n' = n,\ \nu' = \nu,\ \nabla\nu\wedge(\boldsymbol{d}^a - \boldsymbol{d}^{a\prime}) = 0,\quad \nu\in\mathcal{F}. \tag{22}$$

Given Σ, call the set of states $\Sigma'(\neq\Sigma)$ which solves (22) the states *neutrally related* to Σ. Thus the question asked earlier in this section may be rephrased as follows; if Σ and Σ' are neutrally related to one another, is it true that there exists a diffeomorphism $\boldsymbol{u}:\Omega\to\boldsymbol{u}(\Omega)\equiv\Omega$ such that (3) holds (with *replaced by ′)?

EXAMPLE. Let $\Sigma = \{\boldsymbol{e}_a,\ 1,\ \Omega\}$, with $\boldsymbol{e}_1,\ \boldsymbol{e}_2,\ \boldsymbol{e}_3$ a canonical basis of $\mathbb{R}^3$. Then Σ' solves (22) if and only if

$$\boldsymbol{d}^{a\prime} = \nabla\tau^a, \quad \det\nabla\tau^a = 1, \quad \rho' = 1, \tag{23}$$

for some *potential* function $\boldsymbol{\tau} = (\tau^a) : \Omega \to \boldsymbol{\tau}(\Omega)$, arbitrary except for $(23)_2$. If one assumes, in addition, that $\boldsymbol{\tau}$ is 1 - 1, then we have that

$$\text{vol } \Omega = \text{vol } \boldsymbol{\tau}(\Omega). \tag{24}$$

REMARKS

1. The set of states neutrally related to an arbitrary state Σ is completely characterised in [4].
2. In the example above, Σ' is *not* generally an elastic deformation of Σ. To see this, assume the contrary and suppose that there exists a diffeomorphism π such that

$$\nabla\tau^a\left(\boldsymbol{\pi}(\boldsymbol{x})\right) = (\nabla\boldsymbol{\pi})^{-T}\boldsymbol{e}^a, \quad \det(\nabla\tau^a) = 1 \tag{25}$$

and *importantly* $\boldsymbol{\pi}(\Omega) = \Omega$. Then from $(25)_1$, $\boldsymbol{\tau}\cdot\boldsymbol{\pi} =$ identity $+$ constant, and so $\boldsymbol{\tau}(\Omega) = \Omega +$ constant. But this conclusion, that $\boldsymbol{\tau}(\Omega)$ is a translation of Ω, is not ensured by (23). It follows that Σ, Σ' are elastically related if and only if $\boldsymbol{\tau}(\Omega)$ is a translation of Ω, and that generally, Σ and Σ' are related by elastic deformation composed with a rearrangement of the set Ω (to form $\boldsymbol{\tau}(\Omega)$). See [4], [5], [12] for more details regarding this point, and for some remarks regarding the slip mechanism of plasticity.
3. A computation given in [4] shows that equations (22) ensure that the classifying manifolds of Σ, Σ' are *identical.* Thus, given $\boldsymbol{x}_0 \in \Omega$ there is a diffeomorphism $\boldsymbol{u}_{\boldsymbol{x}_0}(\cdot)$ of a neighbourhood $N_{\boldsymbol{x}_0}$ of $\boldsymbol{x}_0$ in Ω such that

$$\boldsymbol{d}'_a\left(\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})\right) = \nabla\boldsymbol{u}_{\boldsymbol{x}_0}(\boldsymbol{x})\boldsymbol{d}_a(\boldsymbol{x}),\ \boldsymbol{x} \in N_{\boldsymbol{x}_0}, \tag{26}$$

and $\boldsymbol{u}(\boldsymbol{x}_0) = \boldsymbol{x}_0$. Moreover, it is shown in [4] that when (22) holds, $(3)_2$ also holds. Hence, neutrally related states are locally elastically related, in the sense that (3) holds *locally.* But neutrally related states are not (globally) elastically related by virtue of remark 2 above.

5. Structure of Crystal States where each of the Scalars $\frac{S^{ab}}{n}$, a, b=1, 2, 3 is Constant

Firstly, when all of the fields $\frac{S^{ab}}{n}$ are constant, those constants may not be prescribed arbitrarily, for

$$\begin{aligned} 0 &= \nabla \cdot (\nabla \wedge \boldsymbol{d}^b) = \nabla \cdot \left\{ (\boldsymbol{d}^a \cdot \nabla \wedge \boldsymbol{d}^b) \boldsymbol{d}_a \right\} \\ &= \nabla \cdot \left(\frac{S^{ab}}{n} n \boldsymbol{d}_a \right) = \frac{1}{2} \frac{S^{ab}}{n} \nabla \cdot (\varepsilon_{ars} \boldsymbol{d}^r \wedge \boldsymbol{d}^s) = \varepsilon_{ars} \frac{S^{ab}}{n} S^{rs} \end{aligned} \tag{27}$$

Then, if one puts

$$C^k_{ij} = \varepsilon_{ijp} \frac{S^{kp}}{n}, \tag{28}$$

it turns out that (28) can be rewritten as

$$C^m_{ij} C^r_{mk} + C^m_{jk} C^r_{mi} + C^m_{ki} C^r_{mj} = 0, \tag{29}$$

which is the Jacobi identity for a three-dimensional Lie algebra. Now, let us aim to find lattice vector fields which are such that each $\frac{S^{ab}}{n}$ is constant. Notice to begin with that the $\frac{S^{ab}}{n}$ are scalars, so if Σ has each $\frac{S^{ab}}{n}$ constant, then so does any state elastically related to Σ. There is then a basic indeterminacy which we may exploit by constructing what Pontryagin [13] calls a canonical system of coordinates of the first kind - in our terminology this amounts to finding a particular state Σ^{mc} which has the structure of a Lie group in the following sense; suppose $\Sigma^{mc} = \{\boldsymbol{D}_a, \boldsymbol{\mathcal{P}}, \Omega^{mc}\}$, then

$$\boldsymbol{D}_a (\boldsymbol{u}(\boldsymbol{x})) = \nabla \boldsymbol{u}(\boldsymbol{x}) \boldsymbol{D}_a(\boldsymbol{x}), \tag{30}$$

where $\boldsymbol{u}(\boldsymbol{x}) \equiv \boldsymbol{\xi}(\boldsymbol{x}, \ \boldsymbol{y})$, with $\xi(\cdot, \cdot)$ the composition function for the Lie group which has structure constants C^k_{ij}, and $\boldsymbol{y}$ chosen arbitrarily, subject to domain requirements. The lattice vectors $\boldsymbol{D}_a$ behave as if they are embedded in the elastic deformation defined by the mapping $\boldsymbol{u}(\cdot) \equiv \boldsymbol{\xi}(\cdot, \boldsymbol{y})$ (so Σ^{mc} is locally elastically related to itself, as one might forsee by an application of the theorem of Section 3 to *copies* of Σ^{mc}). I refer the reader to [10], [11] for the explicit construction of Σ^{mc} in some cases. If, for example, $\left(\frac{S^{ab}}{n}\right) = \boldsymbol{\alpha} \otimes \boldsymbol{\alpha}, \ \boldsymbol{\alpha} \in I\!R^3$, it turns out that $\boldsymbol{\xi}(\cdot, \cdot)$ is affine in both arguments and that one can then show that

$$\boldsymbol{\xi}(\boldsymbol{e}_a, \boldsymbol{x}) = \boldsymbol{x} + \boldsymbol{D}_a(\boldsymbol{x}). \tag{31}$$

It seems to me that this relation is important, for it connects continuum and discrete models of the crystal. On the one hand the fields $\boldsymbol{D}_a$, the structure constants C_{ij}^k and the composition function $\boldsymbol{\xi}$ relate to the description of the crystal as a continuum. On the other hand, the mapping $\boldsymbol{x} :\rightarrow \boldsymbol{x} + \boldsymbol{D}_a(\boldsymbol{x})$ represents the idea that if there is an 'atom' located at a point $\boldsymbol{x} \in \mathbb{R}^3$, then there is also an atom at the point $\boldsymbol{x} + \boldsymbol{D}_a(\boldsymbol{x})$, $a = 1, 2, 3$, and so on. *Iterations* of this mapping thereby generate sets of points which are consistent with the continuum description. One can, in some cases, catalogue these sets of points explicitly, but I do not have the space to describe the various intriguing possibilities here. Broadly, following what has become common practice in nonlinear elasticity, in deciding on material symmetries of constitutive functions, the idea is now to examine the symmetries of this discrete set of atoms and to assume that these symmetries also apply in the continuum setting, so to delimit, prudently, a class of functionals appropriate for studying the mechanics of solid crystals.

Finally, I have not touched upon the subtle connection between continuum and discrete representations of the mass density function in this context.

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