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FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On defective crystallography

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

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SUPPOSE that a solid crystal derives from a perfect (Bravais) lattice of atoms, so that the set of rearrangements of the points of this lattice provides symmetries of the crystal. In the elasticity theory appropriate to such a crystal, it is traditional to assert that the corresponding strain energy density function has invariance properties related to a (proper) subset of these symmetries. Here I discuss similar issues in the context of the continuum mechanics of smoothly defective crystals, focusing on planar distributions of defects.

1. Introduction

I DISCUSS issues related to material symmetry for defective crystals. Experience with perfect crystals shows that choosing an appropriate symmetry group for constitutive functions that govern the mechanics is a subtle procedure. To be specific, one usually chooses a point group of orthogonal transformations as symmetry group for the strain energy function (say) of a cubic crystal in continuum mechanics, even though this is not the full group of symmetries of a cubic lattice, and even though a cubic lattice is not a continuum. So it is natural to try to understand the issues related to the choice of symmetry group first of all in the context of perfect crystals, before proceeding to the defective case, and I outline relevant concepts in Sec. 2 of the paper. Aside from the purely pragmatic reason that calculations based on the point group symmetries perform reasonably well in linear elasticity theories, there is just one logical reason that I know to prefer these groups. That reason derives from a calculation of FONSECA [6], which shows that

- for a strain energy function w with symmetry group corresponding to the full set of rearrangements of a cubic lattice,
- with A the class of Lipshitz deformations $\mathbf{u}$ defined on a region Ω satisfying homogeneous boundary condition $\mathbf{u} = F\mathbf{x}$, $F \in M^+_{3\times 3}$, $\mathbf{x} \in \partial\Omega$,

$$\inf_A \int_\Omega w(\nabla \mathbf{u}) = |\Omega|\, \phi(\det F) \tag{1.1}$$

for some $\phi : \mathbb{R}^+ \to \mathbb{R}$ (see also CHIPOT [2]). This implies, loosely, that a perfect crystal cannot sustain shear stresses in equilibrium, and it is a rigorous result

which one must somehow reconcile with the fact that the shear strength of real crystals is nonzero. Various options present themselves for consideration:

- no real crystal is perfect, but if for the sake of argument we suppose that some real crystal is perfect,
- equilibria do not correspond to infima of an energy functional of the form given above, but if equilibria do correspond to such an infimum,
- the choice of symmetry of group for the energy function is incorrect.

In this paper, responding in part to these three options:

- In Sec. 2, I describe aspects of perfect crystal symmetry, concentrating on two-dimensional crystals, for the sake of simplicity;
- In Sec. 3, I introduce geometric variables which categorize crystals which are not perfect, but which are *defective*, and focus on special cases where the defectiveness of the crystals is uniform;
- For *planar* defective crystals, in Sec. 4, I discuss the construction of discrete sets of points which are compatible with the continuum description of the crystal, and derive some symmetries of these sets of points. Then I suggest that some of these symmetries should be taken over to the continuum model. It turns out that relevant symmetries are determined by the dislocation density tensor, so that the symmetries depend on position only to the extent that the dislocation density depends on position.

2. Perfect crystal symmetry

Let

$$\Lambda(\mathbf{v}_a) = \left\{\mathbf{x} \in \mathbb{R}^2;\ \ \mathbf{x} = m_a\mathbf{v}_a,\ \ m_1, m_2 \in \mathcal{Z}\right\} \tag{2.1}$$

be a real 2-dimensional lattice with the two basis vectors $\mathbf{v}_1$, $\mathbf{v}_2$ linearly independent. Note that $\Lambda(\mathbf{v}_a) = \Lambda(\mathbf{v}'_0)$ if and only if

$$\mathbf{v}'_a = m_{ab}\mathbf{v}_b\,, \tag{2.2}$$

where (m_{ab}) is a matrix of integers with $|\det(m_{ab})| = 1$. If one regards the points of $\Lambda(\mathbf{v}_a)$ as embedded in a continuum, then any deformation of the continuum, with deformation gradient denoted F, which has the property that

$$F\mathbf{v}_a = \mathbf{v}'_a\,, \tag{2.3}$$

maps the lattice onto itself, in the sense that if $x \equiv m_a\mathbf{v}_a \in \Lambda(\mathbf{v}_a)$, then

$$F\mathbf{x} = F(m_a\mathbf{v}_a) = m_a(F\mathbf{v}_a) = m_a\mathbf{v}'_a \in \Lambda(\mathbf{v}'_a) \equiv \Lambda(\mathbf{v}_a). \tag{2.4}$$

So there is an infinite number of deformations which rearrange the discrete points of the lattice $\Lambda(\mathbf{v}_a)$.

The apparatus of traditional crystallography is directed at the classification of subgroups of the set of rearrangements of the points of $\Lambda(\mathbf{v}_a)$. Specifically, one considers those rearrangements (m_{ab}) such that

$$F\mathbf{v}_a = m_{ab}\mathbf{v}_b\,, \tag{2.5}$$

where F is orthogonal. If $\{\mathbf{v}_a\}$ is given, the orthogonal transformations that satisfy (2.5), for some (m_{ab}) of the appropriate form, make up the *point group* of $\Lambda(\mathbf{v}_a)$, and the rearrangements that satisfy (2.5) for some orthogonal F make up the *lattice group* of $\Lambda(\mathbf{v}_a)$ (see ERICKSEN [5], PARRY [16], ZANZOTTO [19]).

If one deals, in nonlinear elasticity, with strain energy density functions of the form $\tilde{w}(\mathbf{v}_a)$ and accepts that the individual atoms which correspond to the points of $\Lambda(\mathbf{v}_a)$ are indistinguishable, then it is reasonable to require that

$$\tilde{w}(\mathbf{v}'_a) = \tilde{w}(\mathbf{v}_a), \tag{2.6}$$

whenever (2.2) holds. In addition, it is common to assume that there exist fixed vectors $\mathbf{V}_a$ such that

$$\mathbf{v}_a = T\mathbf{V}_a\,, \tag{2.7}$$

where T is the macroscopic deformation gradient which governs the behaviour of material line elements relative to an appropriate reference configuration. This is called the Cauchy–Born hypothesis (see ZANZOTTO [20] for comments on this hypothesis). With (2.6) and (2.7), define $w(T)$ by

$$w(T) = \tilde{w}(\mathbf{v}_a). \tag{2.8}$$

Then the symmetry property (2.6) gives

$$\begin{aligned} w(T) = \tilde{w}(\mathbf{v}_a) = \tilde{w}(m_{ab}\mathbf{v}_b) = \tilde{w}(m_{ab}T\mathbf{V}_b) = \tilde{w}(Tm_{ab}\mathbf{V}_b) \\ = \tilde{w}(TS\mathbf{V}_b) = w(TS), \end{aligned} \tag{2.9}$$

if one writes, following (2.5),

$$S\mathbf{V}_b = m_{ab}\mathbf{V}_b\,. \tag{2.10}$$

One might call the orthogonal S which satisfy (2.10) elements of the point group of the reference lattice $\Lambda(\mathbf{V}_a)$, so the symmetries of the corresponding strain energy density include those given by $w(T) = w(TS)$, with S in this point group, as in (2.9). However there is no logical reason, *a priori*, to exclude those non-orthogonal solutions S of (2.10) which correspond to the symmetry property (2.6) (but recall Fonseca's calculation) and concentrate just on the relevant point group.

Finally, classical theorems of invariant theory (GREEN and ADKINS [8], WEYL [18]) give representations of the solutions $w(\cdot)$ of (2.9) for an arbitrary point

group. Solutions $\tilde{w}(\cdot)$ of (2.6), on the other hand, are constructed by finding a fundamental domain $\mathcal{D}$ with the properties that

(i) if $\{\mathbf{v}_a\} \in \mathcal{D}$, then there is no other point of $\mathcal{D}$ which has the form $\{m_{ab}\mathbf{v}_b\}$,
(ii) each $\{\mathbf{v}'_a\}$ may be written as $\{m_{ab}\mathbf{v}_b\}$ with $\{\mathbf{v}_b\} \in \mathcal{D}$.

There are various ways of constructing such a domain $\mathcal{D}$;

- PARRY [13] and PITTERI [17] give (equivalent) geometric and analytic methods of finding $\mathcal{D}$.
- One can conveniently rephrase the problem in complex form, see PARRY [16]. This method has various other advantages, too.
- CONWAY and SLOANE [3] give arithmetical ways of solving the problem.

3. Defective crystals

In this section I replace the basis vectors $\{\mathbf{v}_a\}$ which generate the perfect Bravais lattice $\Lambda(\mathbf{v}_a)$ by *lattice vector fields* $\{\mathbf{d}_a(\cdot)\}$ which are imagined to characterize the internal structure of the crystal, see DAVINI and PARRY [4], PARRY [14], FONSECA and PARRY [7].

A *state* Σ of the crystal consists of three lattice vector fields $\mathbf{d}_1(\mathbf{x})$, $\mathbf{d}_2(\mathbf{x})$, $\mathbf{d}_3(\mathbf{x})$ defined at each point $\mathbf{x}$ of a region Ω, thus

$$\Sigma = \{\mathbf{d}_a(\cdot), \quad a = 1,2,3; \Omega\}. \tag{3.1}$$

For brevity I write henceforward $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$. It is assumed that $\mathbf{d}_1(\mathbf{x})\cdot\mathbf{d}_2(\mathbf{x})\wedge\mathbf{d}_3(\mathbf{x}) \neq 0$, for all $\mathbf{x} \in \Omega$, so there exist *dual lattice vector fields* $\mathbf{d}^1(\mathbf{x}), \mathbf{d}^2(\mathbf{x}), \mathbf{d}^3(\mathbf{x})$ with the property that $\mathbf{d}^a(\mathbf{x})\cdot\mathbf{d}_b(\mathbf{x}) = \delta^a_b$. Two states $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$, $\Sigma^* = \{\mathbf{d}^*_a(\cdot), \Omega^*\}$ are *elastically related* to each other if there exists an invertible smooth mapping $\mathbf{u} : \Omega \to \Omega^* = \mathbf{u}(\Omega)$ such that

$$\begin{aligned} \mathbf{d}^*_a(\mathbf{u}(\mathbf{x})) &= \nabla\mathbf{u}(\mathbf{x})\mathbf{d}_a(\mathbf{x}), \qquad \text{or} \\ \mathbf{d}^{a*}(\mathbf{u}(\mathbf{x})) &= [\nabla\mathbf{u}(\mathbf{x})]^{-T}\mathbf{d}^a(\mathbf{x}), \qquad a = 1,2,3, \quad \mathbf{x} \in \Omega. \end{aligned} \tag{3.2}$$

It is evident from (3.2) that the Burgers integral $\oint_C \mathbf{d}^a(\mathbf{x})\cdot\mathbf{dx}$, C a contour, is an *elastic invariant integral*, in the sense that

$$\oint_{\mathbf{u}(C)=C^*} \mathbf{d}^{a*}(\mathbf{y})\cdot\mathbf{dy} = \oint_C \mathbf{d}^a(\mathbf{x})\cdot\mathbf{dx} \tag{3.3}$$

if Σ and Σ^* are elastically related to each other. It is shown in [4] that there is an infinite number of elastic invariant integrals, and that there is a finite functional basis for the corresponding set of densities. Central to the proof of these results is the notion of a (real-valued) *scalar* defined on a state $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$. Thus

$$\mu_\Sigma(\mathbf{x}) \equiv \mu(\mathbf{x}, \mathbf{d}_a(\mathbf{x}), \quad \nabla\mathbf{d}_a(\mathbf{x}), \quad \nabla^2\mathbf{d}_a(\mathbf{x}), \quad \ldots) \tag{3.4}$$

is a *scalar* if wherever Σ and Σ^* are elastically related to each other, then

$$\mu_\Sigma(\mathbf{x}) = \mu_{\Sigma^*}(\mathbf{u}(\mathbf{x})). \tag{3.5}$$

From (3.5) one can regard the scalars as some kind of internal variables for plasticity theory, since they are transported unchanged in any elastic deformation. The prototypical examples of such a function $\mu_\Sigma(\cdot)$ are the nine functions

$$\frac{\mathbf{d}^a \cdot \nabla \wedge \mathbf{d}^b}{\det\{\mathbf{d}^a\}} \equiv \frac{S^{ab}}{n} \tag{3.6}$$

which are lattice components of the dislocation density tensor, cf. KONDO, BILBY, KRÖNER [9, 1, 10, 11]. (In (3.6), I *define* $S^{ab} = \mathbf{d}^a \cdot \nabla \wedge \mathbf{d}^b$, $n = \det\{\mathbf{d}^a\} = \mathbf{d}^1 \cdot \mathbf{d}^2 \wedge \mathbf{d}^3$). From (3.2) and (3.5) it is clear that $\oint_C \mu_\Sigma(x)\mathbf{d}^a(\mathbf{x}) \cdot \mathbf{dx}$ is also an elastic invariant integral, one can also easily show that $\int_V \mu_\Sigma(\mathbf{x}) n \, dV$ is an elastic invariant integral.

Slips and rearrangements enter this theory if one enquires how two different given states are connected when all the elastic invariant integrals match in the two states. It is clear that if the two states are elastically related, then these integrals match; the point is that there are other changes of state which preserve the integrals which are *not* elastic deformations. It is shown in PARRY [14] that these changes of state can be interpreted as *slip* in surfaces (say) where lattice vector fields are constant. Also there is some compatibility requirement on states that allow slip (partial integrability). Again in [14] it is shown that if there is a non-elastic change of state, from $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$ to $\Sigma' = \{\mathbf{d}'_a(\cdot), \Omega\}$, preserving the integral invariants, then

$$\nabla \wedge (\mathbf{d}^a - \mathbf{d}^{a\prime}) = 0, \qquad \nu n = \nu' n', \qquad \nabla\nu \wedge (\mathbf{d}^a - \mathbf{d}^{a\prime}) = 0, \tag{3.7}$$

whenever

$$\nu \in \mathcal{F} \equiv \left\{ 1, \frac{S^{ab}}{n}(\cdot), \ (\mathbf{d}_c \cdot \nabla)\frac{S^{ab}}{n}(\cdot); \ a, b, c = 1, 2, 3 \right\}. \tag{3.8}$$

In fact these last equations (3.7) are *necessary and sufficient* that *all* integral invariants match in the two states Σ, Σ'. I do not discuss the derivation of these equations here, nor the requirement that Σ, Σ' are defined over the same region Ω (this is not a restriction, in fact). In [15] I use a theorem of Cartan, in a form quoted by OLVER [12], to derive abstract properties of states Σ which are such that (3.7) has a nontrivial solution for Σ' (that is, a solution with $\Sigma' \neq \Sigma$). I choose to display the relevant properties of such states, here, only in the particular case where the nine scalars S^{ab}/n are *constant* throughout Ω.

THEOREM 1. *States Σ such that* (3.7) *has a solution $\Sigma' \neq \Sigma$ are locally diffeomorphic to a state Σ^{mc} which has the structure of a (local) Lie group with structure constants $\varepsilon_{ijk}(S^{\ell k}/n)$.*

NOTES

1. States $\Sigma = \{\mathbf{d}_a(\cdot), \Omega\}$, $\Sigma^{mc} = \{\mathbf{D}_a(\cdot), \Omega^{mc}\}$ are locally diffeomorphic if and only if for each $\mathbf{x}_0 \in \Omega$ there exists a neighbourhood $N_{\mathbf{x}_0}$ of $\mathbf{x}_0$ in Ω and a diffeomorphism $\mathbf{u}_{\mathbf{x}_0} : N_{\mathbf{x}_0} \to \mathbf{u}_{\mathbf{x}_0}(N_{\mathbf{x}_0})$ such that $\mathbf{D}_a(\mathbf{u}_{\mathbf{x}_0}(\mathbf{x})) = \nabla \mathbf{u}_{\mathbf{x}_0}(\mathbf{x})\mathbf{d}_a(\mathbf{x})$, $\mathbf{x} \in N_{\mathbf{x}_0}$.

2. I say that Σ^{mc} has the structure of a (local) Lie group $\mathcal{G}$ with structure constants $\varepsilon_{ijk}(S^{\ell k}/n)$ if and only if

$$\mathbf{D}_a(\zeta(\mathbf{X}, \mathbf{Y})) = \nabla_{\mathbf{X}} \zeta(\mathbf{X}, \mathbf{Y}) \mathbf{D}_a(\mathbf{X}), \qquad \mathbf{Y} \in \Omega^{mc}, \tag{3.9}$$

where ζ is the composition function for $\mathcal{G}$, so that if $g(X)$, $g(Y)$ are group elements corresponding to the parametrization by points $\mathbf{X} \in \Omega^{mc}$, then $g(\zeta(\mathbf{X}, \mathbf{Y})) = g(\mathbf{X})g(\mathbf{Y})$. If one fixes $\mathbf{Y}$ in (3.9) and puts $\zeta(\mathbf{X}, \mathbf{Y}) \equiv \mathbf{u}_{\mathbf{Y}}(\mathbf{X})$, then (3.9) becomes

$$\mathbf{D}_a(\mathbf{u}_{\mathbf{Y}}(\mathbf{X})) = \nabla_{\mathbf{X}} \mathbf{u}_{\mathbf{Y}}(\mathbf{X}) \mathbf{D}_a(\mathbf{X}), \tag{3.10}$$

so that Σ^{mc} is locally diffeomorphic to *itself*. This result could be derived from [4]; what is new here is the identification of the local elastic deformation which takes Σ^{mc} to itself as the composition function for $\mathcal{G}$. States which allow slip, then, have the Lie group structure given by (3.9). The corresponding dual vector fields $\mathbf{D}^a(\mathbf{x})$ are called left-invariant in the Lie group literature, they are the Maurer–Cartan fields (forms) on the group.

4. Symmetry of crystals with planar distributions of defects

Now I focus on the particular case where

$$\mathbf{d}_1 = \mathbf{d}_1(x_1, x_2), \qquad \mathbf{d}_2 = \mathbf{d}_2(x_1, x_2), \qquad \mathbf{d}_3 = \mathbf{e}_3 . \tag{4.1}$$

In this case only two of the components of the dislocation density may be nonzero and they are

$$S^{31}/n = -\lambda, \qquad S^{32}/n = \mu. \tag{4.2}$$

I assume that λ and μ are constant (so that the theorem of Sec. 3 applies), and I show elsewhere that there is no loss of generality (so far as the subsequent discussion is concerned) in assuming that

$$\mathbf{d}_1 = \mathbf{e}_1 + \mu \mathbf{x}, \qquad \mathbf{d}_2 = \mathbf{e}_2 + \lambda \mathbf{x}. \tag{4.3}$$

To decide on the symmetry of relevant constitutive functions, I ask if there are any sets of points naturally associated with these vector fields. One might have the view that if there is an "atom" of the crystal at the point $\mathbf{x}$, then there must also be an atom at the point $\mathbf{x} + \mathbf{d}_a(\mathbf{x})$ (by virtue of an interpretation of the vectors $\mathbf{d}_a$ as vectors joining "nearest neighbour" atoms, perhaps). However

this notion does not have appropriate invariance properties, in general, and it is better to assert that if there is an atom at $\mathbf{x}$, then there is also an atom at $\mathbf{x}_a$ where $\mathbf{x}_a$ is defined by

$$\dot{\mathbf{y}} = \mathbf{d}_a(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{x}, \qquad \mathbf{y}(t_a) = \mathbf{x}_a\,, \tag{4.4}$$

where the numbers t_1, t_2, t_3 are to be prescribed. A set of points which is consistent with this interpretation of the vector fields should have the properties:

(i) iterations (4.4) of points in the set remain in the set,

(ii) there is a (nonzero) minimum distance between points in the set.

The numbers $\{t_a\}$ determine whether or not these properties are satisfied. I give results just for the simple case where

$$\mu t_1 = \lambda t_2 = \ln 2, \qquad t_3 = 1 \tag{4.5}$$

(more general results will be given elsewhere). In this case, from (4.4), notice that $\dot{\mathbf{y}} = \mathbf{d}_1(\mathbf{y}) = \mathbf{e}_1 + \mu\mathbf{y}$ may be written as $(\mathbf{y} + \mu^{-1}\mathbf{e}_1)^{\cdot} = \mu(\mathbf{y} + \mu^{-1}\mathbf{e}_1)$, so $\mathbf{y} + \mu^{-1}\mathbf{e}_1 = e^{\mu t}(\mathbf{x} + \mu^{-1}\mathbf{e}_1)$. Thus $(\mathbf{x}_1 + \mu^{-1}\mathbf{e}_1) = 2(\mathbf{x} + \mu^{-1}\mathbf{e}_1)$ and in the same way $\mathbf{x}_2 + \lambda^{-1}\mathbf{e}_2 = 2(\mathbf{x} + \lambda^{-1}\mathbf{e}_2)$. Then, one can show that the set of points

$$S(\mathbf{x}) = \left\{\mathbf{y} : \mathbf{y} = 2^m\left(\mathbf{x} + \frac{\mathbf{e}_1}{\mu}\right) + n\left(\frac{\mathbf{e}_1}{\mu} - \frac{\mathbf{e}_2}{\lambda}\right) - \frac{\mathbf{e}_1}{\mu}, \quad m \in \mathcal{Z}^+, \quad n \in \mathcal{Z}\right\}, \tag{4.6}$$

has properties (i) and (ii) above, and so the rearrangements of $S(\mathbf{x})$ are of interest. Note that $S(\mathbf{x})$ can be rewritten as

$$S(\mathbf{x}) = \left\{\mathbf{y} : \mathbf{y} = 2^m\frac{\mathbf{d}_1(x)}{\mu} + n\left(\frac{\mathbf{d}_1(\mathbf{x})}{\mu} - \frac{\mathbf{d}_2(\mathbf{x})}{\lambda}\right) - \frac{\mathbf{e}_1}{\mu}, \quad m \in \mathcal{Z}^+, \quad n = \mathcal{Z}\right\}. \tag{4.7}$$

Let

$$\tilde{\mathbf{d}}_1 = \mathbf{d}_1 + \mu\boldsymbol{\nu}, \qquad \tilde{\mathbf{d}}_2 = \mathbf{d}_2 + \lambda\boldsymbol{\nu}, \qquad \boldsymbol{\nu} = \frac{\mathbf{d}_1}{\mu} - \frac{\mathbf{d}_2}{\lambda}, \qquad \tilde{\boldsymbol{\nu}} = \frac{\tilde{\mathbf{d}}_1}{\mu} - \frac{\tilde{\mathbf{d}}_2}{\lambda} \quad (\equiv \boldsymbol{\nu}).$$

Then $S(\mathbf{x})$ can also be recast as

$$S(\mathbf{x}) = \left\{\mathbf{y} : \mathbf{y} = 2^m\frac{\tilde{\mathbf{d}}_1(\mathbf{x})}{\mu_1} + n\tilde{\boldsymbol{\nu}} - \frac{\mathbf{e}_1}{\mu}, \quad m \in \mathcal{Z}^+, \quad n \in \mathcal{Z}\right\}, \tag{4.8}$$

so that the mapping $\mathbf{d}_a \to \tilde{\mathbf{d}}_a$ gives a rearrangement of $S(\mathbf{x})$, But $\tilde{\mathbf{d}}_a = \gamma_{ab}\mathbf{d}_b$, where

$$(\gamma_{ab}) = \begin{pmatrix} 2 & -\mu/\lambda & 0 \\ \lambda/\mu & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4.9}$$

Recalling (4.2), one sees that this symmetry of the set of points $S(\mathbf{x})$ depends on the dislocation density tensor.

If, now, one seeks to identify symmetries of an objective strain energy density function

$$w = w(\mathbf{d}^a \cdot \mathbf{d}^b, \ S^{ab}/n), \tag{4.10}$$

which have the form $\mathbf{d}_a \to \gamma_{ab}\mathbf{d}_b \equiv \widetilde{\mathbf{d}}_b$, notice first of all that $\widetilde{\mathbf{d}}^a = (\gamma^{-T})^{ab}\mathbf{d}^b$, so that $\widetilde{S}^{ab} = (\gamma^{-\top})^{ab}S^{cd}(\gamma^{-1})^{db}$ and $\widetilde{n} = (\det\gamma)^{-1}n$. The point of view that has been taken in this paper suggests that the *particular* mapping corresponding to (4.9) be taken as a symmetry of the energy density, as it preserves a relevant set of points. But for this particular mapping, and for the particular dislocation density (4.2) one calculates that

$$\widetilde{S}^{ab}/\widetilde{n} = S^{ab}/n, \tag{4.11}$$

so that the symmetry derived by consideration of the rearrangements of the discrete set of points preserves the (continuum) dislocation density tensor (moreover, the symmetry is independent of the point $\mathbf{x}$ which parameterizes $S(\mathbf{x})$). Finally, one deduces that the energy density must, at least, satisfy

$$w\left(\mathbf{d}^a \cdot \mathbf{d}^b, \ S^{ab}/n\right) = w\left(\widetilde{\mathbf{d}}^a \cdot \widetilde{\mathbf{d}}^b, \ S^{ab}/n\right), \tag{4.12}$$

where $\widetilde{\mathbf{d}}^a = (\gamma^{-\top})^{ab}\mathbf{d}^b$ and (γ) is given by (4.9), which generalizes (2.6) to the case of a defective crystal.

References

1. B.A. BILBY, *Continuous distributions of dislocations*, [in:] Progress in Solid Mechanics, I. SNEDDON [Ed.], vol. 1, North-Holland, Amsterdam 1960.
2. M. CHIPOT, *Hyperelasticity for crystals*, European J. Applied Math., **1**, 113–129, 1990.
3. J.H. CONWAY and N.J.A. SLOANE, *Low-dimensional lattices. VI. Voronoi reduction of three-dimensional lattices*, Proc. R. Soc. London, **A 436**, 55–68, 1992.
4. C. DAVINI and G.P. PARRY, *A complete list of invariants for defective crystals*, Proc. R. Soc. London, **A 432**, 341–365, 1991.
5. J.L. ERICKSEN, *Weak martensitic transformations in Bravais lattices*, Arch. Rat. Mech. Anal., **107**, 23–36, 1989.
6. I. FONSECA, *Variational methods for elastic crystals*, Arch. Rat. Mech. Anal., **97**, 189–220, 1987.
7. I. FONSECA and G.P. PARRY, *Equilibrium configurations of defective crystals*, Arch. Rat. Mech. Anal., **120**, 245–283, 1992.
8. A.E. GREEN and J.E. ADKINS, *Large elastic deformations*, 2nd edition, Clarendon Press, Oxford 1970.
9. K. KONDO, *Non-Riemannian geometry of imperfect crystals from a macroscopic viewpoint*, [in:] RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Science by Means of Geometry, K. KONDO [Ed.], vol. 1, Gakuyusty Bunken Fukin-Day, Tokyo 1955.

10. E. KRÖNER, *Allgemeine Kontinuumstheorie der Versetzungen und Eigenspannungen*, Arch. Rat. Mech. Anal., **4**, 273–334, 1960.
11. E. KRÖNER, *Continuum theory of defects*, [in:] Physics of Defects, R. BALLIAN, M. KLÉMAN and J.-P POIRER [Eds.], Amsterdam: North-Holland 1981.
12. P. OLVER, *Invariants, equivalance and symmetry*, Cambridge University Press, Cambridge 1995.
13. G.P. PARRY, *On the elasticity of monatomic crystals*, Math. Proc. Camb. Phil. Soc., **80**, 189–211, 1976.
14. G.P. PARRY, *Defects and rearrangements in crystals*, [in:] Defects and Anelasticity in the Characterization of Crystalline Solids, Applied Mechanics Division, L.M. BROCK [Ed.], **148**, American Society of Mechanical Engineers, New York 1992.
15. G.P. PARRY, *Elastic-plastic decompositions of defect-preserving changes of state in solid crystals*, [in:] Trends in Applications of Mathematics to Mechanics, Pitman Monographs and Surveys in Pure and Applied Mathematics, M.D.P. MONTEIRO MARQUES and J.F. RODRIGUES [Eds.], **77**, Longman, Harlow, Essex 1995.
16. G.P. PARRY, *Low dimensional lattice groups*, Arch. Rat. Mech. Anal. [to appear].
17. M. PITTERI, *Reconciliation of local and global symmetries of crystals*, J. Elasticity, **14**, 175–190, 1984.
18. H. WEYL, *Classical groups*, 2nd edition, Princeton University Press, Princeton, New Jersey 1973.
19. G. ZANZOTTO, *Weak and symmetry-breaking transitions in simple lattices*, preprint 1996.
20. G. ZANZOTTO, *The Cauchy-Born hypothesis, nonlinear elasticity and mechanical twinning in crystals*, Acta Crystallographica, **A 52**, 839–849, 1996.

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