Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 1 (2000)
Geom., Cont. and Micros., I

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POLYCRYSTALLINE MICROSTRUCTURE

Abstract. Polycrystals are often modelled as Cosserat continua, the crystallographic directions within single crystals being represented through elements of $SO(3)$. To address the problem of an overall representation of a polycrystalline aggregate, following the example of nematics, one may choose an appropriate embedding of $SO(3)$ in a linear space. Some possibilities are explored and a suggestion is made for such a choice.

1. Introduction

1.1. Orientation distribution in polycrystals

A polycrystal is a material body the elements of which comprise each a population of 'specks' having the structure of a single perfect crystal. In the simplest instance all such crystallites are of the same kind, i.e., any two of them can be superposed through a rigid displacement. Thus a reference crystallite can be chosen and a lattice orientation function can be assigned to describe the polycrystal's substructure. This approach is standard in metallurgical analyses and the problem of determining the orientation function is of industrial import.

The sketch above pertains to a particular range of observation scales. Actually no lattice at all can be defined within dislocations cores, while, observing metals at low temperature and at a scale significantly larger than the average dislocation spacing, a grain pattern appears. The lattice orientation function is constant on regions of finite volume (the bulk of grains) and jumps across their boundaries.

When observations at a scale much larger than the largest grain size are involved no account is taken of grain shapes and the polycrystal is described simply through an orientation distribution function on the basis of probabilistic assumptions. The need arises for a global description through a distribution of lattice orientations.

Thus when computations at a scale much larger than the largest grain size are involved, one may wish to consider body elements which include many hundreds of grains and are characterised by a whole distribution of lattice orientations. The question arises as to the constitutive nature of the interactions between neighbouring body elements; it seems reasonable to start by assuming that these interactions depend on the first moment of the distribution and thus on some 'average' orientation of the crystals within the material elements, and that these averages evolve according to general rules described by multifield theories, whereas evolutions of the orientation distribution function deep within the element be described on the basis of a multivariable theory (cf. [4, 5, 7, 8, 18]).

*We thank our friend Fulvio Lazzeri for useful suggestions. This research is part of the programme "Modelli Matematici per la Scienza dei Materiali" of the Italian Ministero dell'Università e della Ricerca Scientifica e Tecnologica.

In the case of polycrystals the manifold $\mathcal{M}$ of 'deep' states, *l'éspace profond* of [7], is a subset of $SO(3)$ (symmetry arguments may make $\mathcal{M}$ a proper subgroup of $SO(3)$) and, at each point $x \in \mathcal{E}$, $\mathcal{M}$ is endowed with the structure of a probability space, so that each $\mu \in \mathcal{M}$ is a random variable with probability density, say, γ (the orientation distribution function). Assuming that self-effects be weakly non-local in $\mathcal{M}$, in the sense of [14], evolution equations of general type can be found for γ, whereas interactions among neighbours in $\mathcal{E}$ occur through some kind of average over $\mathcal{M}$ based on γ.

To achieve that average a device, simple to use, could be invoked. Whitney's theorem affirms that a linear space $\mathcal{S}$, of dimension $2m+1$, exists within which the manifold $\mathcal{M}$, of dimension m, can be embedded. The embedding is not unique and there are even cases where the embedding is feasible in a linear space of dimension lower than $2m+1$ (e.g., $SO(3)$, of dimension 3, can be embedded in a 5-dimensional linear space). However the essential point is that $\mathcal{S}$ exists and, in it, averages can be evaluated in a straightforward manner; they fall, generally, outside the image $\widehat{\mathcal{M}}$ of $\mathcal{M}$ in $\mathcal{S}$, and fill altogether the convex hull $\mathcal{H}$ of that image. Within $\mathcal{H}$ complete disorder is represented by the average of a uniform distribution on $\mathcal{M}$.

1.2. General remarks on continuum models

The possible teaming up, for certain tasks, of a multifield and a multivariable theory has led one of us to advance the remarks which follow [16]; we recall them here because they are strictly relevant and give to our present proposal a very general setting.

Multifield theories are based on the classical space-time $\mathcal{E}\times\mathcal{T}$. Fields $\nu : \mathcal{E}\times\mathcal{T} \to \mathcal{N}$ ($\mathcal{N}$ a manifold of 'substructures') enrich the 'natural' classic description which invokes only bijections $\mathcal{E} \to \mathcal{E}$ at each instant. Interactions between elements are supposed to have short range in $\mathcal{E}$ *à la Cauchy*, though the nature of these interactions depends now, by duality arguments, on the greater kinematic richness of the model.

Multivariable theories start from a wider representation of physical space, obtained by adding to standard placements in $\mathcal{E}$ a set $\mathcal{M}$ of 'deep' placements μ. Interactions range now between neighbours in $\mathcal{E} \times \mathcal{M}$, but the duality is usually narrow. These theories take the components μ^α of μ as extra independent variables beside the place variable x (and time if the case requires). They introduce a distribution function $\gamma\,(\mu, x)$ such that $\gamma\,(\mu, x)\,d\mu$ measures the fraction of fragments of the element at x having a value of the substructure falling within the interval $(\mu, \mu + d\mu)$.

In some current research contributions it is assumed that the evolution of γ is totally dictated by the internal state of each element and related to gradients in the variable μ in a sort of weakly nonlocal (on $\mathcal{M}$) mode. Within the element spatial distances do not count, whereas it is easy to believe that two fragments with slightly different values of μ influence one another more than two fragments whose values are, in some measure, distant, irrespective of the exact location of the two fragments within the element. The assumption of an exclusively internal dependence may be sometimes a limiting factor, but this is not so critical in some problems for polycrystalline solids where interelement effects due to spatial gradients are modest, or occur mainly through the agency of macrostress; contrariwise, when studying nematics and hyperfluids [10], one perceives easily the depth of influence of certain constraining boundary conditions.

One way to fix the loophole: find somehow an average value of μ over each element and imagine such average influenced by the averages in neighbouring elements in the same way as happens in less deep theories where all fragments in an element lead to the same value of the substructural variable. Perhaps extract some 'frame' or background from the averages and, if objectivity commands, describe the internal distributions γ and their internal evolution against that background. Judicious steps are always required to arrive at a proper and significant definition of average. Previous embedding of the manifold $\mathcal{M}$ in a linear space $\mathcal{S}$ of higher dimension is always possible (in dimension $2m+1$, by the already quoted theorem of Whitney); then calculation of averages is straightforward.

Actually reference to $\widehat{\mathcal{M}}$, as a hypersurface in $\mathcal{S}$, rather then to the intrinsic manifold $\mathcal{M}$, if managed with care, makes many developments easier; correspondingly $\mathcal{S}$ may take the place of $\mathcal{N}$, again if prudence is exercised to avoid breaches of objectivity. Known concepts and relations may be imported with advantage from available multifield theories.

Thus, for our present task, the matter of embedding $SO(3)$ in a linear space is an essential prerequisite and becomes the core of our developments. To pave the way and make it even more evident, we pause to consider first the simpler, and in part already well established, case of nematic liquid crystals.

2. The example of nematics

In the theory of nematic liquid crystals $\mathcal{M}$ is the manifold of directions, hence of dimension 2. Whitney's embedding can be realised in a linear space of dimension 5. Each direction is put first into one-to-one correspondence with the tensor $n \otimes n - \frac{1}{3}I$, where n is any one of the two unit vectors having the required direction and I is the identity. All those tensors belong to the linear space (with dimension 5) of the symmetric traceless tensors; one of them, say N, will be the average when the element contains molecules with varying degree of orientation. The principal axes of N provide the frame upon which details regarding the distribution of orientations can be assigned. Still, already the eigenvalues of $N + \frac{1}{3}I$, call them λ_i determine two parameters which describe essential traits of the distribution: the degree of prolation s (called also, by Ericksen, degree of orientation) in $\left[-\frac{1}{2}, 1\right]$:

$$s = 3\left(\frac{1}{2}\prod_{i=1}^{3}\lambda_i\right)^{1/3}$$

and the degree of triaxiality in [0, 1]

$$\beta = 3^{1/2}2^{1/3}\left|\prod_{i=1}^{3}\left(\lambda_i - \lambda_{i+1}\right)\right|^{1/3}.$$

Perfect ordering corresponds to the values $s = 1$, $\beta = 0$; 'melting' of the liquid crystal occurs when both parameters vanish.

Many problems have been solved satisfactorily using N as a substructural variable and writing for it an appropriate evolution equation which involves the gradient of N in physical space (for a partial analysis in this direction see [2] and [12]; a fuller study is in a forthcoming paper by Biscari and Capriz).

However, if the details of the distribution of directions $\gamma(n)$ become relevant for specific problems, then the following further steps must be taken. An evolution equation for γ must be proposed, expressing its 'conservation' (the total of γ over $\mathcal{N}$ must always equal to 1); here a suggestion of Muschik [3, 17] may be accepted though modified so as to admit also an influence on γ of N and of the gross displacement gradient F.

Ultimately one comes to the equation

$$\frac{\partial\gamma}{\partial\tau} + \operatorname{div}_N(\gamma\dot{n}) + (\operatorname{grad}_N\gamma)\cdot\dot{N} + (\operatorname{grad}_F\gamma)\cdot\dot{F} = 0\,,$$

where gradients enter along the manifolds $\mathcal{M}$ and $\mathcal{N}$. Actually if $n \otimes n$, rather than n, had been chosen as a variable, then div_n would have been substituted by the appropriate surface divergence along $\widehat{\mathcal{M}}$ in $\mathcal{S}$.

The balance equation above, exhaustive though it be in very special cases, must be supplemented in general by a 'deep' balance equation, which, in statics, may express a minimality condition for the energy connected with a certain choice of $\gamma(N)$ and of its gradient on $\widehat{\mathcal{M}}$. Alternatively, there may be steady states of deformation (e.g. of shearing) dominated by some sort of viscous action which must be itself balanced (for matching developments in the theory of polycrystals see [4, 6, 7, 9]).

3. Embedding of $SO(3)$ in $\mathbb{R}^5$

The so called 'easy Whitney embedding theorem' (cfr. [19]) proves that $SO(3)$ can, as any compact (Hausdorff C^r, $2 \leq r \leq \infty$) three dimensional manifold, be embedded in $\mathbb{R}^7$, though embeddings into linear spaces of smaller dimension may be possible.

It has been proved that $SO(3)$ cannot be embedded into $\mathbb{R}^4$ (cfr. [11]), while an embedding into $\mathbb{R}^5$ is known. The latter result can be shown through a chain of differentiable inclusions: $SO(3)$ can be included into $S^2 \times S^2$ associating with each element of the orthogonal matrix any two column vectors of it:

$$\begin{bmatrix} c_1^{(1)} & c_1^{(2)} & c_1^{(3)} \\ c_2^{(1)} & c_2^{(2)} & c_2^{(3)} \\ c_3^{(1)} & c_3^{(2)} & c_3^{(3)} \end{bmatrix} \in SO(3) \to (c^{(1)}, c^{(2)}) \in S^2 \times S^2$$

One of the two unit 2-spheres S^2 can be included into $]0, +\infty[\times\mathbb{R}^2$:

$$c^{(2)} \in S^2 \to (\xi c_1^{(2)} + \zeta, \xi c_2^{(2)}, \xi c_3^{(2)}) \in]0, +\infty[\times\mathbb{R}^2\,,$$

with $0 < \xi < \zeta$; then

$$S^2 \times (]0, +\infty[\times\mathbb{R}^2) = (S^2\times]0, +\infty[) \times \mathbb{R}^2 \approx (\mathbb{R}^3 - \{0\}) \times \mathbb{R}^2 \subset \mathbb{R}^5\,.$$

Notice that $S^2\times]0, +\infty[$ is diffeomorphic to $\mathbb{R}^3 - \{0\}$ as it can be shown, e.g., choosing coordinates (ϑ, ϕ) on S^2 and taking the corresponding polar coordinates $c^{(1)} = (\sin\phi\cos\vartheta, \sin\phi\sin\vartheta, \cos\phi)$ on $\mathbb{R}^3 - \{0\}$:

$$(\vartheta, \phi, \rho) \in S^2\times]0, +\infty[\to (\rho\sin\phi\cos\vartheta, \rho\sin\phi\sin\vartheta, \rho\cos\phi) \in \mathbb{R}^3 - \{0\}\,.$$

We thus have the embedding:

$$\left[c_j^{(i)}\right] \in SO(3) \to$$

$$(c_1^{(1)}(\xi c_1^{(2)} + \zeta), c_2^{(1)}(\xi c_1^{(2)} + \zeta), c_3^{(1)}(\xi c_1^{(2)} + \zeta), \xi c_2^{(2)}, \xi c_3^{(2)}) \in \mathbb{R}^5\,.$$

It can be shown that the conditions $\|c^{(1)}\| = 1$ and $\|c^{(2)}\| = 1$, and the condition $c^{(1)} \cdot c^{(2)} = 0$ correspond respectively to the equations ($x \in \mathbb{R}^5$):

$$(1) \qquad \begin{aligned} &(\|x\|^2 - \xi^2 - \zeta^2)^2 + 4\zeta^2(x_4^2 + x_5^2) = 4\xi^2\zeta^2 \,, \\ &x_1(\|x\|^2 - \xi^2 - \zeta^2) + 2\zeta(x_2x_4 + x_3x_5) = 0 \,. \end{aligned}$$

4. Embedding a subgroup of $SO(3)$ into Sym_0

The embedding recalled in Sect. 3 from texts in differential geometry does not appear to have intrinsic character required on principle for its use in a physical theory; the appropriate alternative is the introduction of a symmetric tensor of a special class to denote a particular lattice orientation.

We must emphasise, however, at the outset that application of the theorem to our physical context will be legitimate only when a set of three mutually orthogonal directions (no arrow!), each endowed with a different characteristic length, exist having an immediate physical significance in the description of crystallites (e.g. the edges of the elementary cell if the crystalline system is orthorombic). Call $\{m^{(i)} \mid i \in \{1, 2, 3\}\}$, $\|m^{(1)}\| < \|m^{(2)}\| < \|m^{(3)}\|$, the vectors representing a crystallite, their sign being immaterial to the physical description of the crystallite, normalized to make

$$\sum_{i=1}^{3} (m^{(i)})^2 = 1 \,.$$

A polycrystal is a cluster of such crystallites, each uniquely identified through the proper orthogonal tensor Q giving the rotation from a set of reference unit vectors $\{c^{(i)}\}$ to the crystallite's unit vectors $\{m^{(i)}/\|m^{(i)}\|\}$ modulus rotations of π about any $c^{(i)}$; call $\mathcal{M} \subset SO(3)$ the subgroup of such rotations.

Now let us define the following map from the same set of crystallites to the linear space of symmetric tensors

$$S(\{m^{(i)}\}) = \sum_{i=1}^{3} m^{(i)} \otimes m^{(i)} \,;$$

for all $\{m^{(i)}\}$ it is $\operatorname{tr} S = 1$, $\operatorname{tr} S^2 = \sum_{i=1}^{3} (m^{(i)})^4$, and $\det S = \prod_{i=1}^{3} (m^{(i)})^2$.

There is a one to one differentiable map between the set of crystallites and the elements of Sym which verify the conditions listed above; in particular any tensor S verifying these conditions has three distinct eigenvalues $(m^{(i)})^2$, with the corresponding eigenvectors parallel to the vectors $m^{(i)}$. The spectral decomposition of such a tensor S is thus

$$S(\{m^{(i)}\}) = Q D^2 Q^T \,,$$

where D is the diagonal matrix

$$D := \begin{bmatrix} \|m^{(1)}\| & 0 & 0 \\ 0 & \|m^{(2)}\| & 0 \\ 0 & 0 & \|m^{(3)}\| \end{bmatrix} .$$

Therefore

$$\mathcal{M} \approx \left\{ S \in Sym \;\middle|\; \operatorname{tr} S = 1, \; \operatorname{tr} S^2 = \sum_{i=1}^{3} (m^{(i)})^4, \; \det S = \prod_{i=1}^{3} (m^{(i)})^2 \right\} ,$$

and one can suggest the embedding in the affine space:

$$\mathcal{M} \hookrightarrow \mathcal{S} \equiv \{S \in Sym \mid \operatorname{tr} S = 1\} \ .$$

REMARK 1. Chosen any reference the general element of $\mathcal{S}$ is represented by

$$S = \begin{bmatrix} x_1 & x_5 & x_4 \\ x_5 & x_2 & x_3 \\ x_4 & x_3 & 1 - x_1 - x_2 \end{bmatrix} ,$$

i.e., by a mapping $\mathcal{S} \to \mathbb{R}^5$. The conditions $\operatorname{tr} S^2 = \sum_{i=1}^{3} (m^{(i)})^4$ and $\det S = \prod_{i=1}^{3} (m^{(i)})^2$, can be written in coordinates (cfr. equations (1)):

$$\|x\|^2 + x_1 x_2 - x_1 - x_2 + 1 = \textstyle\sum_{i=1}^{3} (m^{(i)})^4 \ ,$$
$$(x_1 x_2 - x_5^2)(1 - x_1 - x_2) - x_1 x_3^2 - x_2 x_4^2 + 2 x_3 x_4 x_5 = \textstyle\prod_{i=1}^{3} (m^{(i)})^2 \ ,$$

representing the image $\widehat{\mathcal{M}}$ of $\mathcal{M}$ in $\mathcal{S}$.

5. Conclusion

A distribution of orthorhombic crystals can be represented through the mean orientation defined as:

$$\tilde{S} := \int_{SO(3)} \gamma(Q) S(Q) \, d(SO(3)) \ .$$

If the distribution is one of perfect order, with all crystals oriented as some $\widehat{Q}$, then $\tilde{S} = S(\widehat{Q})$ has three distinct eigenvalues and the corresponding eigenvectors represent the axes of the crystallite. Contrariwise, if the disorder is complete, then $\tilde{S}$ is spherical and no preferred axis can be assigned to the average representation of the distribution of crystals. Intermediate conditions are clearly possible, with the axial optical properties of the aggregate corresponding to the number of distinct eigenvalues of $\tilde{S}$.

We have thus taken the first essential step for a convenient portrait of a polycrystal, a step which opens the way for a rigourous connection between the theory of continua with microstructure as displayed in [13] and the theory of 'deep' space proposed in [4] with direct metallurgical applications in mind.

References

[1] BISCARI P., CAPRIZ G. AND VIRGA E., *Biaxial nematic liquid crystal*, in: "Boundary-value problems for partial differential equations and applications", (Eds. C. Baiocchi and J.L. Lions), Masson, Paris 1993.

[2] BISCARI P. AND CAPRIZ G., *Optical and statistical anisotropy in nematics*, Rend. Acc. Lincei Matematica **4** (1993), 307–313.

[3] BLENK S., EHRENTRAUT H. AND MUSCHIK W., *A continuum theory for liquid crystals describing different degrees of orientational order*, Liquid Crystals **14** 4 (1993), 1221–1226.

[4] BROCATO M., *Un modèle thermo-mécanique de polycristal pour l'étude des bandes de cisaillement*, Ph. D. Dissertation, ENPC, Paris 1994.

[5] BROCATO M., EHRLACHER A. AND TAMAGNY P., *Cinematica dei continui eterogenei*, Atti XII Convegno Nazionale AIMETA, Napoli 1995, 105–110.

[6] BROCATO M., EHRLACHER A. AND TAMAGNY P., *A two dimensional polycrystal model in a 'deep' space representation*, Meccanica **30** (1995), 641–663.

[7] BROCATO M., *Un modèle mécanique de polycristal*, Presses de l'Ecole Nationale des Ponts et Chaussées, Paris 1996.

[8] BROCATO M., EHRLACHER A. AND TAMAGNY P., *Focal-shift and polycristal models—from the continuum with microstructure to a deep continuum*, Applied Sciences-Especially Mathematics, ZAMM - Z. Angew. Math. Mech. **76** S4 (1996), 117–120.

[9] BROCATO M. AND AIFANTIS E. C., *A theory of plasticity based on globalization of microscopic constitutive assumptions*, in: "Constitutive and damage modeling of inelastic deformation and phase transformation" (Ed. A.S. Khan) Proc. of Plasticity'99, Cancun (Mexico), Neat Press, Fulton, Mariland USA 1999, 701–704.

[10] BROCATO M. AND CAPRIZ G., *Spin fluids and hyperfluids*, Rend. Dip. Mat. Univ. Pisa 2000 and Atti XIV Convegno Nazionale AIMETA, Como (Italy), Oct. 1999, CD-ROM.

[11] BROGLIA F. AND LUMINATI D., *Connected sum of compact analytic hypersurfaces*, Ann. di Mat. Pura ed Appl. **173** 4 (1997), 203–211.

[12] CALDERER M. C. AND LIU C., *Poiseuille flow of nematic liquid crystals*, The Eringen Symposium dedicated to Pierre-Gilles de Gennes, Pullman, WA, 1998, Int. J. Engrg. Sci. **38** 9-10 (2000), 1007–1022.

[13] CAPRIZ G., *Continua with microstructure*, Springer-Verlag, New York 1989.

[14] CAPRIZ G. AND GIOVINE P., *Weakly non local effects in mechanics*, Rend. Dip. Mat. Univ. Pisa 1999.

[15] CAPRIZ G., *Continua with substructure. Part I*, Physical Mesomechanics **3** 4 (2000), 5–13.

[16] CAPRIZ G., *Continua with substructure. Part II*, Physical Mesomechanics **3** 6 (2000), 37–48.

[17] EHRENTRAUT H., MUSCHIK W. AND PAPENFUSS C., *Mesoscopically derived orientation dynamics of liquid crystals*, J. Non-Equilib. Thermodyn. **22** (1997), 285–298.

[18] EHRLACHER A., TAMAGNY P. AND BROCATO M., *Change of scale in media with microstructure*, in: "Geometry, Continua and Microstructure"', (Ed. G. A. Maugin), Hermann, Paris 1999, 131–143.

[19] MORRIS W. HIRSCH, *Differential topology*, Springer-Verlag, New York 1976.

[20] TAMAGNY P., *Les milieux à microstructure; approches par la méthode des puissances virtuelles*, Ph. D. Dissertation, ENPC, Paris 1996.

AMS Subject Classification: 74A30, 74A40, 74A60.

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