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

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ARE CONTINUOUS DISTRIBUTIONS OF INHOMOGENEITIES IN LIQUID CRYSTALS POSSIBLE?

Abstract. Within a theory of liquid-crystals-like materials based on a generalized Cosserat-type formulation, it is shown that continuous distributions of inhomogeneities may exist at the microstructural level.

1. Introduction

In the conventional theories of liquid crystals, the free-energy density is assumed to be a function of a *spatial* vector field and its spatial gradient. Starting from the pioneering work of Frank [6], various improvements were proposed by Leslie [9] and by Ericksen [4] [5]. A different point of view was advocated by Lee and Eringen [7] [8], as early as 1972, when considering a liquid criystal within the framework of the theory of materials with internal structure. The main difference between these points of view is that the second approach emphasizes the dependence of the constitutive equations on the *mappings* between vectors or tensor fields, rather than on their values alone. This mapping-dependence is essential not only for sustaining continuous distributions of inhomogeneities, but also, as shown by Maugin and Trimarco [10], for the proper setting of a definition of Eshelby stresses. The general connection between these two aspects of material behaviour is described in [3].

2. The generalized Cosserat medium

A *generalized Cosserat body* (GCB) consists of the frame bundle of an ordinary body $\mathcal{B}$. In other words, a GCB is a body plus the collection of all its local frames at each point. Denoting by X^I ($I = 1, 2, 3$) and x^i ($i = 1, 2, 3$) Cartesian coordinate systems for the body $\mathcal{B}$ and for physical space, respectively, a configuration of a GCB consists of the twelve independent functions:

$$x^i = x^i(X^J)$$
$$H^i{}_I = H^i{}_I(X^J)$$

where H^i_I represents the mapping of the frames attached at point X^J. It is important to stress that the ordinary deformation gradient $F^i_I = \frac{\partial x^i}{\partial X^I}$ and the mapping H^i_I are of the same nature, but represent two independent vector-dragging mechanisms.

A GCB is *hyperelastic* of the first grade if its material response can be completely characterized by a single scalar ("strain-energy") function:

$$W = W(F^i{}_I, H^i{}_I, H^i{}_{I,J}; X^K)$$

*Partially supported by the Natural Sciences and Engineering Research Council of Canada, and DGI-CYT (Spain) (Project PB97-1257).

where comma subscripts denote partial derivatives. Under a change of reference configuration of the form

$$Y^A = Y^A(X^J)$$
$$H^A{}_I = H^A{}_I(X^J)$$

where the indices A, B, C are used for the new reference, the energy function changes to:

$$\begin{aligned} W &= W'(F^i{}_A, H^i{}_A, H^i{}_{A,B}; Y^C) \\ &= W(F^i{}_A F^A{}_I, H^i{}_A H^A{}_I, H^i{}_{A,B} F^B{}_J H^A{}_I + H^i{}_A H^A{}_{I,J}; X^K(Y^C)) \end{aligned} \tag{1}$$

Notice the special form of the composition law for the derivatives of H^i_I.

Generalizing Noll's idea of uniformity [11], by taking into account the composition laws in Equation (1), one can show [1] [2] that in terms of an archetypal energy function

$$W_c = W_c(F^i{}_\alpha, H^i{}_\alpha, H^i{}_{\alpha\beta})$$

where Greek indices are used for the archetype, a GCB is *uniform* (namely, it is made of "the same material" at all points) if there exist three uniformity fields of tensors $P^I{}_\alpha(X^J)$, $Q^I{}_\alpha(X^J)$ and $R^I{}_{\alpha\beta}(X^J)$ such that the equation

$$W(F^i{}_I, H^i{}_I, H^i{}_{I,J}; X^K) = W_c(F^i{}_I P^I{}_\alpha, H^i{}_I Q^I{}_\alpha, H^i{}_{I,J} P^J{}_\beta Q^I{}_\alpha + H^i{}_I R^I{}_{\alpha\beta})$$

is satisfied identically for all non-singular $F^i{}_I$ and $H^i{}_I$ and for all $H^i{}_{I,J}$. *Homogeneity* (global or local) follows if, and only if, there exists a (global or local) reference configuration such that these fields become trivial.

3. The liquid-crystal-like model

We call a *liquid-crystal-like model* (LCM) a material whose internal structure can be represented by the deformation of one or more vector or tensor fields. More specifically, we say that a GCB is of the LCM type if a nowhere-zero material vector field $\mathbf{D} = D^I \mathbf{E}_I$ and a material tensor field $\mathbf{A} = A^I{}_J \mathbf{E}_I \otimes \mathbf{E}^J$ exist such that the energy density function depends on its arguments in the following way:

$$W = W(F^i{}_I, H^i{}_I, H^i{}_{I,J}; X^K) = f(F^i{}_I, H^i{}_I D^I, H^i{}_{I,J} D^I + H^i{}_I A^I{}_J; X^K) \tag{2}$$

where we have used the letter f to denote the new functional dependence.

To clarify the rationale behind this definition, we consider first the particular case of a reference configuration in which $\mathbf{D}(\mathbf{X})$ constitutes a parallel unit vector field and $\mathbf{A}(\mathbf{X})$ vanishes identically. We can then write (for that particular reference configuration, if it exists) that

$$W = f(F^i{}_I, H^i{}_I D^I, (H^i{}_I D^I)_{,J}; X^K)$$

This constitutive equation is unable to detect any difference between different deformations of triads that happen to map the director into the same vector in space. In other words, all that matters is the resulting vector and its gradient, just as in the "conventional" theory of liquid crystals, and it is in this sense that Equation (2) constitutes a generalization. More importantly, when seen under this light, the tensor $\mathbf{A}$ no longer appears as an artificial construct, but as the natural outcome of describing the manner in which the conventional archetype has been inserted in the body in a pointwise fashion.

It is apparent that the particular form of the constitutive law adopted for an LCM must entail certain *minimal symmetries*, namely, certain local changes of reference configuration that are indistinguishable as far as the material response is concerned. In addition, an LCM may have other non-generic symmetries, but here we are interested in deriving those symmetries that are already inherent in the definition. Now, any symmetry of a GCB consists of a triple $\{G, K, L\}$ satisfying:

$$\begin{aligned} f(F^i{}_J, H^i{}_J D^J, H^i{}_{M,N} D^M + H^i{}_M A^M{}_N; X^K) = \\ f(F^i{}_I G^I{}_J, H^i{}_I K^I{}_J D^J, (H^i{}_{I,J} G^J{}_N K^I{}_M + H^i{}_I L^I{}_{MN}) D^M + H^i{}_I K^I{}_M A^M{}_N; X^K) \end{aligned}$$

for all non-singular $F^i{}_I$ and $H^i{}_I$ and for all $H^i{}_{I,J}$. Since we are looking for minimal symmetries, namely, those stemming from the particular dependence assumed on H and its gradient, we set G equal to the identity. It then follows that the energy function will have the same values for all K and L satisfying the following identities:

$$H^i{}_J D^J = H^i{}_I K^I{}_J D^J$$

and

$$H^i{}_{M,N} D^M + H^i{}_M A^M{}_N = H^i{}_{I,N} K^I{}_M D^M + H^i{}_I L^I{}_{MN} D^M + H^i{}_I K^I{}_M A^M{}_N$$

for all non-singular $F^i{}_I$ and $H^i{}_I$ and for all $H^i{}_{I,J}$. It follows immediately that the minimal symmetries are those satisfying the following conditions:

$$K^I{}_J D^J = D^I \tag{3}$$

and

$$L^I{}_{MN} D^M = (\delta^I{}_M - K^I{}_M) A^M{}_N \tag{4}$$

The first condition is the obvious one: the energy function at a point remains invariant under any change of reference configuration which leaves the director at that point unchanged. In other words, the matrix K has the director as an eigenvector corresponding to a unit eigenvalue. The second condition, on the other hand, is far from obvious and could not have been predicted except by means of the kinematically based method we have used. Note that in the particular case in which the tensor field $\mathbf{A}$ is zero, the right-hand side of the second condition vanishes. It is not difficult to show by a direct calculation that the collection of all the symmetries satisfying the above two conditions forms a group $\mathcal{G}_{min}$, which we will call the *minimal symmetry group* of any LCM, under the multiplication law given by Equation (1).

Although not strictly necessary, we will adopt as the *LCM archetype* a point whose constitutive law is of the form

$$W_c = W_c(F^i{}_\alpha, H^i{}_\alpha, H^i{}_{\alpha\beta}) = f_c(F^i{}_\alpha, H^i{}_\alpha D^\alpha, H^i{}_{\alpha\beta})$$

namely, we adopt $A^\alpha{}_{\beta\gamma} = 0$ at the archetype. According to the general prescription for uniformity, then, fields $P^I{}_\alpha(X^K)$, $Q^I{}_\alpha(X^K)$ and $R^I{}_{\alpha\beta}(X^K)$ must exist such that:

$$\begin{aligned} & W(F^i{}_I, H^i{}_I, H^i{}_{I,J}; X^K) \\ & = W_c(F^i{}_I P^I{}_\alpha, H^i{}_I Q^I{}_\alpha, H^i{}_{I,J} P^J{}_\beta Q^I{}_\alpha + H^i{}_I R^I{}_{\alpha\beta}) \\ & = f_c(F^i{}_I P^I{}_\alpha, H^i{}_I Q^I{}_\alpha D^\alpha, (H^i{}_{I,J} P^J{}_\beta Q^I{}_\alpha + H^i{}_I R^I{}_{\alpha\beta}) D^\alpha) \end{aligned}$$

It is a straightforward matter to verify that the resulting function W has the requisite form:

$$W(F^i{}_I, H^i{}_I, H^i{}_{I,J}; X^K) = f(F^i{}_I, H^i{}_I D^I, (H^i{}_{I,J} D^I + H^i{}_I A^I{}_J))$$

where

$$D^I = Q^I{}_\alpha D^\alpha$$

and

$$A^I{}_J = R^I{}_{\alpha\beta}(P^{-1})^\beta{}_J D^\alpha$$

Indeed

$$\begin{aligned} & f_c(F^i{}_I P^I{}_\alpha, H^i{}_I Q^I{}_\alpha D^\alpha, (H^i{}_{I,J} P^J{}_\beta Q^I{}_\alpha + H^i{}_I R^I{}_{\alpha\beta}) D^\alpha) \\ &= f_c(F^i{}_I P^I{}_\alpha, H^i{}_I D^I, P^J{}_\beta (H^i{}_{I,J} D^I + H^i{}_I A^I{}_J)) \\ &= f(F^i{}_I, H^i{}_I D^I, H^i{}_{I,J} D^I + H^i{}_I A^I{}_J; X^K) \end{aligned}$$

Under a change of reference configuration we know that the tensor field $A^I{}_J$ transforms to

$$A^A{}_B = (H^A{}_{I,J} D^I + H^A{}_I A^I{}_J)(F^{-1})^J{}_B$$

and we ask the question: does there exist a change of reference configuration leading to an identically vanishing $A^A{}_B$ in an open neighbourhood of a point? It is not difficult to show that a sufficient condition for this local homogeneity requirement to take place is that:

$$A^I{}_J = D^I{}_{,J}$$

identically in that neighbourhood. Indeed, if that is the case, we can write:

$$A^A{}_B = (H^A{}_I D^I)_{,J} (F^{-1})^J{}_B$$

Therefore, any change of reference configuration of the form

$$Y^A = Y^A(X^K)$$

$$H^A{}_I = (Q^{-1})^\alpha{}_I \delta^A{}_\alpha$$

will do the job. We conclude then that the local homogeneity of an LCM body is guaranteed, in addition to the ordinary condition of homogeneity of the macromedium, by the equation

$$A^I{}_J = D^I{}_{,J} \tag{5}$$

describing the compatibility of the liquid crystal superstructure. If, however, the underlying macromedium is homogeneous but condition (5) is violated, we have a genuine distribution of inhomogeneities at the microstructural level. On the other hand, it can be shown that the two conditions taken together are not only sufficient, but also necessary, for local homogeneity of an LCM uniform body whose symmetry group is minimal. This fact holds true even though the minimal symmetry group is continuous. More surprisingly, perhaps, the same conclusion holds even when the macromedium is a genuine liquid, namely, when its symmetry group is the whole unimodular group.

Assume that we have a reference configuration that is homogeneous as far as the underlying macromedium is concerned and in which the director field is unit and parallel. The only source of inhomogeneity left is, therefore, a smooth second-order tensor field $\mathbf{A}(\mathbf{X})$. By the polar decomposition theorem, this field can be seen geometrically as a field of ellipsoids, whose axes and eccentricities vary smoothly from point to point. In principle, then, we have a situation equivalent to that of a standard liquid crystal, except that the standard ellipsoids of orientational distribution are now replaced by the ellipsoids arising form the inhomogeneity of the microstructure. These last ellipsoids are manifest, as already noted, even if the director field is perfectly unitary and parallel! The typical optical patterns, whose beautiful curvy shapes have become associated in popular imagination with liquid crystals, and usually explained as a manifestation of the variation of the mean orientational order of the molecules, could therefore be explained equivalently by the presence of continuous distributions of inhomogeneities.

4. Concluding remarks

We have shown that, at least in principle, it is possible to formulate a theory of liquid-crystal-like uniform bodies that admit continuous distributions of inhomogeneities. The main ingredient of this theory is the inclusion of maps, and derivatives thereof, between whole fibres of the principal frame bundle of the underlying body. This stands in contrast with the conventional theory, which recognizes only the transformation of a single vector field and its derivative. Although the treatment of a liquid crystal as some kind of generalized Cosserat body is not new, the way in which a particular director field is made to enter the formulation is different from previous formulations. Instead of imposing a constitutive symmetry upon a standard Cosserat medium, we emphasize a kinematic motivation as a rationale for constraining the constitutive functional to a particular form, and only then derive a-posteriori results for the minimal symmetry group. These results differ form the a-priori counterparts in [7] and [8] in the rather complicated symmetry requirement for the microstructural component, a requirement that is absent in the a-priori statement. But it is precisely this condition that allows for the existence of legitimate microstructural inhomogeneities. Further mathematical details of the theory are now under investigation, including differential-geometric implications.

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AMS Subject Classification: 73B25, 53C10.

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