

Mesoscopic continuum mechanics applied to liquid crystals

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Beyond the usual 5-field theory (basic fields: mass density, velocity, internal energy), additional variables are needed for the unique description of complex media. Beside the conventional method of introducing additional fields by their balances, an other procedure, the mesoscopic theory, is here discussed and applied to liquid crystals.

1 Introduction

Continuum mechanics is based on the balance equations of mass, momentum, angular momentum or spin, total or kinetic energy and internal energy. Additionally, one has to consider the balance of entropy for taking into account the second law. In non-relativistic physics, all these balances are defined on time and position (\mathbf{x}, t) . Beyond the quantities whose balance equations are mentioned above, complex materials need more variables for their unique description. Examples for these additional quantities are internal variables, order and damage parameters, Cosserat triads, directors and alignment and conformation tensors.

In principle, there are two possibilities to include these additional quantities into the continuum theoretical description: One can introduce additional fields and their balance equations defined on (\mathbf{x}, t) as in the case of the balance for the macroscopic director, or the additional quantities, the so-called mesoscopic variables, are introduced as variables extending space-time to the so-called mesoscopic space. This description introducing the mesoscopic space is called the mesoscopic theory. According to its construction, the dimension of the mesoscopic space is equal to the number of the mesoscopic variables plus four.

The balances of mass, momentum, etc., can be easily written down on the mesoscopic space because only the number of dimensions changed in comparison with the usual balances on space-time. The different values of the mesoscopic variables in a given volume element are described by a mesoscopic distribution function (MDF), representing the statistical tool of the mesoscopic description. The moments of the MDF, generated by integration over the mesoscopic variables, are additional macroscopic fields which are beyond the fields appearing in the usual balance equations.

2 The mesoscopic concept

In principle there are two possibilities to include additional quantities into the continuum theoretical description (Muschik et al., 2000). One can introduce additional fields and their balance equation defined on $(\mathbf{x}, t) \in R^3 \times R^1$, or the additional quantities are introduced as variables extending $R^3 \times R^1$ to the so-called mesoscopic space on which now the balances of mass, momentum, etc., are defined. The first possibility for describing complex materials by introducing additional fields has a long history in continuum mechanics. Starting out with the first contribution of the Cosserat brothers (1907, 1909), the development of mechanics of generalized continua is lasting since today (Eringen and Şuhubi, 1964; Eringen and Kafarda, 1976; Capriz, 1989). The second possibility introducing the mesoscopic space is called the *mesoscopic concept* which stems historically from the theory of liquid crystals (DeGennes and Prost, 1993; Ericksen, 1960; Leslie, 1965; Eringen and Lee, 1974; Stephen and Straley, 1974; Eringen, 1978; Hess, 1975) by taking the orientation distribution function of the molecules into consideration (Condiff and Brenner, 1969; Blenk et al. 1991, 1993).

As discussed above, the mesoscopic concept introduces the *mesoscopic space*

$$(\mathbf{m}, \mathbf{x}, t) \in \mathcal{M} \times R^3 \times R^1 \quad (1)$$

on which the balances are defined. Here $\mathbf{m} \in \mathcal{M}$ is a set of *mesoscopic variables* which is an element of a suitable manifold \mathcal{M} on which an integration can be defined.

Beyond the use of additional variables \mathbf{m} , the mesoscopic concept introduces a statistical element, the so-called *mesoscopic distribution function* (MDF) $f(\mathbf{m}, \mathbf{x}, t)$ generated by the different values of the mesoscopic variables of the molecules in a volume element

$$f(\mathbf{m}, \mathbf{x}, t) \equiv f(\cdot), \quad (\cdot) \equiv (\mathbf{m}, \mathbf{x}, t) \in \mathcal{M} \times R^3 \times R^1. \quad (2)$$

The MDF is defined on the mesoscopic space $\mathcal{M} \times R^3 \times R^1$ describing the distribution of \mathbf{m} in a volume element around \mathbf{x} at time t , and therefore it is always normalized

$$\int f(\mathbf{m}, \mathbf{x}, t) d\mathcal{M} = 1. \quad (3)$$

3 Local mesoscopic balances

Starting out with a usual local balance equation on space-time $R^3 \times R^1$

$$\frac{\partial}{\partial t} \mathbf{X}(\mathbf{x}, t) + \nabla_x \cdot [\mathbf{v}(\mathbf{x}, t) \mathbf{X}(\mathbf{x}, t) - \mathbf{Q}(\mathbf{x}, t)] = \Sigma(\mathbf{x}, t), \quad (4)$$

we introduce the mesoscopic part by replacing $R^3 \times R^1$ with $\mathcal{M} \times R^3 \times R^1$ and by adding the differentiated part belonging to \mathcal{M} . Thus, we obtain the shape of a *local mesoscopic balance*

$$\frac{\partial}{\partial t} \mathbf{X}(\cdot) + \nabla_x \cdot [\mathbf{v}(\cdot) \mathbf{X}(\cdot) - \mathbf{S}(\cdot)] + \nabla_m \cdot [\mathbf{u}(\cdot) \mathbf{X}(\cdot) - \mathbf{R}(\cdot)] = \Sigma(\cdot). \quad (5)$$

The special balances are obtained by a special physical identification of $\mathbf{X}(\cdot)$, $\mathbf{S}(\cdot)$, $\mathbf{R}(\cdot)$ and $\Sigma(\cdot)$. Beside the mesoscopic velocity $\mathbf{v}(\cdot)$, the *mesoscopic change velocity* $\mathbf{u}(\cdot)$ occurs which is defined as follows

$$(\mathbf{m}, \mathbf{x}, t) \longrightarrow (\mathbf{m} + \mathbf{u}(\cdot) \Delta t, \mathbf{x} + \mathbf{v}(\cdot) \Delta t, t + \Delta t). \quad (6)$$

Especially, we obtain the following local mesoscopic balance equations:

3.1 Mass

$$\frac{\partial}{\partial t} \varrho(\cdot) + \nabla_x \cdot \{\mathbf{v}(\cdot) \varrho(\cdot)\} + \nabla_m \cdot \{\mathbf{u}(\cdot) \varrho(\cdot)\} = 0, \quad (7)$$

3.2 Momentum

$$\begin{aligned} \frac{\partial}{\partial t} [\varrho(\cdot) \mathbf{v}(\cdot)] + \nabla_x \cdot [\mathbf{v}(\cdot) \varrho(\cdot) \mathbf{v}(\cdot) - \mathbf{T}^\top(\cdot)] + \\ + \nabla_m \cdot [\mathbf{u}(\cdot) \varrho(\cdot) \mathbf{v}(\cdot) - \mathcal{T}^\top(\cdot)] = \varrho(\cdot) \mathbf{k}(\cdot), \end{aligned} \quad (8)$$

3.3 Angular momentum and spin

$$\mathbf{M}(\cdot) := \mathbf{x} \times \mathbf{v}(\cdot) + \mathbf{s}(\cdot), \quad \mathbf{s}(\cdot) := \text{mesoscopic specific spin}, \quad (9)$$

$$\begin{aligned} \frac{\partial}{\partial t} [\varrho(\cdot) \mathbf{s}(\cdot)] + \nabla_x \cdot [\mathbf{v}(\cdot) \varrho(\cdot) \mathbf{s}(\cdot) - \mathbf{W}(\cdot)^T] + \\ + \nabla_m \cdot [\mathbf{u}(\cdot) \varrho(\cdot) \mathbf{s}(\cdot) - \mathcal{W}(\cdot)^T] = \varepsilon : \mathbf{T}(\cdot) + \varrho(\cdot) \mathbf{g}(\cdot). \end{aligned} \quad (10)$$

The meaning of the used quantities is as follows:

\mathbf{T} is the mesoscopic Cauchy stress tensor, \mathcal{T} its analogue on the mesoscopic space. \mathbf{k} is the mesoscopic force density and \mathbf{g} the mesoscopic angular momentum exerted by the external forces and momenta on \mathbf{m} . \mathbf{W} is the mesoscopic couple stress and \mathcal{W} its analogue acting on the mesoscopic variables \mathbf{m} .

The mesoscopic balances can be written down very easily because only the number of dimensions differ with respect to the macroscopic balances. Consequently, a setting of new balances is not necessary: the quantities beyond the 5-field theory are included in the mesoscopic space as variables. Of course, not all variables beyond 5-field theory are mesoscopic ones. If there is no mesoscopic distribution function for a special quantity, it is not a mesoscopic variable and cannot be treated with the mesoscopic theory.

4 Macroscopic balances

Finally, we are not interested in the mesoscopic fields, but we have to create macroscopic ones from them. To do so, it is obvious that we have to integrate over the mesoscopic variables to obtain the macroscopic balances

$$\int \dots d\mathcal{M} \longrightarrow \text{macroscopic balance.} \quad (11)$$

Taking into account that the integral over the divergence with respect to the mesoscopic variables vanishes (Blenk et al., 1991)

$$\int \nabla_m \cdot [\dots] d\mathcal{M} = 0, \quad (12)$$

we obtain by integrating the mesoscopic mass balance (7) the following mesoscopic definitions of the macroscopic mass density and velocity

$$\varrho(\mathbf{x}, t) := \int \varrho(\cdot) d\mathcal{M}, \quad \mathbf{v}(\mathbf{x}, t) := \int f(\cdot) \mathbf{v}(\cdot) d\mathcal{M}. \quad (13)$$

In the same way by integrating balances, we obtain the mesoscopic definitions of the macroscopic spin, stress tensor, couple stress, and external momentum

$$\mathbf{s}(\mathbf{x}, t) := \int f(\cdot) \mathbf{s}(\cdot) d\mathcal{M}, \quad (14)$$

$$\mathbf{T}(\mathbf{x}, t) := \int [\mathbf{T}(\cdot) - \mathbf{v}(\cdot) \varrho(\cdot) \mathbf{v}(\cdot)] d\mathcal{M} + \mathbf{v}(\mathbf{x}, t) \varrho(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t), \quad (15)$$

$$\mathbf{W}(\mathbf{x}, t) := \int [\mathbf{W}(\cdot) - \mathbf{s}(\cdot) \varrho(\cdot) \mathbf{v}(\cdot)] d\mathcal{M} + \mathbf{s}(\mathbf{x}, t) \varrho(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t), \quad (16)$$

$$\varrho(\mathbf{x}, t) \mathbf{g}(\mathbf{x}, t) := \int [\varrho(\cdot) \mathbf{g}(\cdot) + \varepsilon : \mathbf{T}(\cdot) - \nabla_m \cdot \mathcal{W}^\top(\cdot)] d\mathcal{M} - \varepsilon : \mathbf{T}(\mathbf{x}, t). \quad (17)$$

Interesting is that the mesoscopic stress tensors and the mesoscopic external moments are not additive forming the macroscopic quantities.

The macroscopic spin balance results from integration of (10) (Blenk and Muschik, 1991)

$$\frac{\partial}{\partial t} [\varrho(\mathbf{x}, t) \mathbf{s}(\mathbf{x}, t)] + \nabla_x \cdot [\mathbf{v}(\mathbf{x}, t) \varrho(\mathbf{x}, t) \mathbf{s}(\mathbf{x}, t) - \mathbf{W}^T(\mathbf{x}, t)] = \quad (18)$$

$$= \varepsilon : \mathbf{T}(\mathbf{x}, t) + \varrho(\mathbf{x}, t) \mathbf{g}(\mathbf{x}, t). \quad (19)$$

With this, the mesoscopic background of the macroscopic balances is elucidated.

5 Entropy balance

Because of the second law which can be formulated only macroscopically, the entropy balance is only interesting in its macroscopic form. It writes

$$\begin{aligned} \frac{\partial}{\partial t} [\varrho(\mathbf{x}, t) \eta(\mathbf{x}, t)] + \nabla_x \cdot [\varrho(\mathbf{x}, t) \eta(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t) + \phi(\mathbf{x}, t)] = \\ = \zeta(\mathbf{x}, t) + \sigma(\mathbf{x}, t). \end{aligned} \quad (20)$$

Here, the fields have the following meaning: $\eta(\mathbf{x}, t)$ = specific entropy, $\phi(\mathbf{x}, t)$ = entropy flux density, $\zeta(\mathbf{x}, t)$ = entropy supply, $\sigma(\mathbf{x}, t)$ = entropy production density. The second law is now expressed by the *dissipation inequality*

$$\sigma(\mathbf{x}, t) \geq 0 \quad (21)$$

which has to be taken into account for writing down constitutive equations (Muschik, 1988; Triani et al., 2008).

6 Distribution function balance

Taking (13)₁ and (3) into account, we obtain

$$\varrho(\cdot) = \varrho(\mathbf{x}, t)f(\cdot). \quad (22)$$

The macroscopic mass balance results from integrating (7) over the mesoscopic variables by taking (12) into account

$$\frac{\partial}{\partial t}\varrho(\mathbf{x}, t) + \nabla_x \cdot \{\mathbf{v}(\mathbf{x}, t)\varrho(\mathbf{x}, t)\} = 0. \quad (23)$$

The macroscopic mass balance induces a differential equation for the mesoscopic distribution function (Muschik et al., 1999)

$$\begin{aligned} \frac{\partial}{\partial t}f(\cdot) + \nabla_x \cdot [\mathbf{v}(\cdot)f(\cdot)] + \nabla_m \cdot [\mathbf{u}(\cdot)f(\cdot)] + \\ + f(\cdot) \left[\frac{\partial}{\partial t} + \mathbf{v}(\cdot) \cdot \nabla_x \right] \ln \varrho(\mathbf{x}, t) = 0. \end{aligned} \quad (24)$$

This *distribution function balance* is a derived one, and consequently, it does not represent an approximation or an ad-hoc equation in the frame of the mesoscopic theory. From the mathematical point of view, (24) is an integro-differential equation due to the appearance of the macroscopic mass density which is an integral over the mesoscopic mass density according to (13)₁. From a physical point of view, (24) is a mean field equation because the mesoscopic distribution function is also determined by the macroscopic mass density.

7 Beyond micropolar media: The order parameters

Beyond the theory of micropolar media, the mesoscopic theory creates additional macroscopic balances of the moments of the MDF. These moments generate the so-called *family of the order parameters*

$$1 = \int f(\cdot) d\mathcal{M}, \quad (25)$$

$$\mathbf{A}(\mathbf{x}, t) := \int f(\cdot) \mathbf{m} d\mathcal{M}, \quad (26)$$

$$\mathbf{a}(\mathbf{x}, t) := \int f(\cdot) \overline{\mathbf{m}\mathbf{m}} d\mathcal{M}, \quad (27)$$

$$\underline{\mathbf{a}}_N(\mathbf{x}, t) := \int f(\cdot) \overline{\mathbf{m} \dots N \text{ times} \dots \mathbf{m}} d\mathcal{M}. \quad (28)$$

Here $\overline{\mathbf{A} \dots \mathbf{B}}$ denotes a symmetric and traceless tensor.

8 An example: Liquid crystals

Liquid crystals consist of needle-shaped molecules. Thus, each molecule points into a special direction which is described by the *microscopic director* \mathbf{n} . Because the molecules are not totally aligned in general, the microscopic directors in a volume element create a distribution function on the unit sphere consisting of the sections of the elongated microscopic directors with the unit sphere. Consequently, the microscopic director is a mesoscopic variable, $\mathbf{n} \equiv \mathbf{m}$, and the mesoscopic procedure can be applied to the microscopic director.

Because here the mesoscopic variables span the 2-dimensional unit sphere S^2 , the mesoscopic space (1) becomes in the case of (nematic) liquid crystals $S^2 \times R^3 \times R^1$. The MDF (2) becomes the *orientation distribution function* of the needle-shaped molecules in the considered volume element. The differential equation of the orientation distribution function is (24). Approximations of this integro-differential equation are used for special cases (Hess, 1975, 1976). The mesoscopic balances become *orientational balances*, the order parameters in sect. 7 are called *alignment tensors*. The alignment tensor of second order (27) is of special interest because it can be measured by optical methods. More details can be found in Muschik et al. (2004).

9 Remarks on constitutive theory

All balance equations contain constitutive equations whose choice makes the system of balances mathematically complete for solution and which determine the material for which the considered system of balance equations is valid. The domain of the constitutive equations is called the *state space* or the *constitutive space* which characterizes the material and which has to be chosen by modelling. The mesoscopic constitutive theory is up to now poorly developed. The reason for that is, that there are different types of state spaces whose final choice is complicated (Ehrentraut, 1996). There are

1: purely mesoscopic state spaces without any mean field influence

$$\mathcal{Z} = (\mathbf{m}, \varrho(\cdot), \overline{\nabla \mathbf{v}(\cdot)}, [\mathbf{u}(\cdot)]^{obj}, \varepsilon(\cdot)), \quad (29)$$

2: purely macroscopic state spaces whose macroscopic variables are defined by a mesoscopic background (Blenk et al., 1992)

$$\mathcal{Z} = (\varrho(\mathbf{x}, t), \overline{\nabla \mathbf{v}(\mathbf{x}, t)}, \varepsilon(\mathbf{x}, t), \mathbf{a}(\mathbf{x}, t), \underline{\mathbf{a}}_4(\mathbf{x}, t), \nabla \mathbf{a}(\mathbf{x}, t)), \quad (30)$$

and finally we have

3: mixed state spaces (Ehrentraut et al., 1997)

$$\mathcal{Z} = (\mathbf{m}, \varrho(\cdot), \overline{\nabla \mathbf{v}(\cdot)}, \nabla_n \ln \varrho(\cdot), \overline{\nabla \mathbf{v}(\mathbf{x}, t)}, \mathbf{a}(\mathbf{x}, t)). \quad (31)$$

Often it is difficult to find out the suitable state space describing a special material. That is one of the reasons why the mesoscopic constitutive theory is poorly developed.

10 Summary

The mesoscopic description is characterized by introducing the mesoscopic space, the product of space-time and the mesoscopic variables, and by introducing the mesoscopic distribution function defined on the mesoscopic space describing the distribution of the values of the mesoscopic variables around a point in space-time. No additional balances for the mesoscopic variables are necessary, because they are introduced as variables of the mesoscopic space and not as additional fields which do need also additional, first of all unknown balances. Instead of them, the mesoscopic description needs a model for the transient behaviour of the mesoscopic variables, the mesoscopic change velocity. Having solved the mesoscopic balances by introducing constitutive equations (a difficult task), the macroscopic quantities, the only which can be measured, are derived by integrating over the mesoscopic variables. By this mesoscopic background, additional macroscopic fields, the moments of the mesoscopic distribution function, the so-called order parameters can be derived which includes the additional mesoscopic information.

Successful application of the mesoscopic theory is always possible, if mesoscopic variables can be defined. Up to now, liquid crystals (Muschik et al., 2004), micro-cracks (Van et al., 2000; Papenfuss et al., 2003) and ferrofluids (Papenfuss et al., 2002) are mesoscopically described.

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