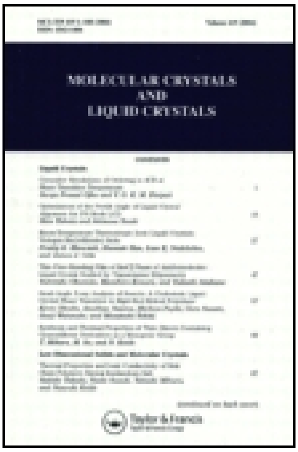

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CONSTITUTIVE THEORY FOR TWO DIMENSIONAL LIQUID CRYSTALS

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Abstract Two dimensional liquid crystal are considered as mathematical surfaces of discontinuity of the bulk fields. The equations of motion for the relevant surface fields in the presence of electromagnetic fields are summarized. These are the mechanical balance equations, Maxwell's equations, and an equation of motion for the second order alignment tensor. The restrictions to constitutive functions implied by the Second Law of Thermodynamics are discussed. The stress tensor can be calculated in the frame of this phenomenological theory. For the alignment production a statistical background is needed, what is very shortly outlined.

INTRODUCTION

Examples for liquid crystals, which can be considered aproximately as two dimensional systems are phase boundaries between liquid crystalline phases, surface layers at walls which are important in displays, and free standing liquid crystalline films which can be produced of a few molecules thickness. Other important examples are lyotropic membranes. But these biologically relevant systems will not be considered here, as they are always multicomponent systems. The boundary will be considered as a mathematical surface of discontinuity of the bulk fields, ignoring any structure perpendicular to the surface [1], [2]. It devides the bulk into the +-region and the - region. The surface is in general curved, and therefore we use a curvilinear system of surface coordinates and a cartesian system in $\mathbb{R}^3$. Tensor components refering to the curvilinear surface coordinate system will be denoted by greek indices, and components with respect to the cartesian coordinate system by latin indices. An index $\perp$ denotes a vector or tensor projected orthogonal to the surface. Summation convention applies to both kinds of indices. $\underline{e}$ is the unit normal to the surface, pointing towards the +-region. τ^1 and τ^2 are the tangential vectors to the surface coordinate lines $\xi^1(\underline{x})$ = constant, $\xi^2(\underline{x})$ = constant:

$$\tau^k_\alpha = \frac{\partial \xi_\alpha}{\partial x_k} \quad . \tag{1}$$

An intrinsic geometrical characterization of the surface is given by the metric $\underline{\underline{g}}$. The second fundamental form (curvature tensor) is denoted with $\underline{\underline{b}}$ with the mean curvature

$$K_M = 1/2tr(\underline{\underline{b}}) \quad . \tag{2}$$

The covariant derivative of the Levi-Civita connection is denoted by ";" and

$$\phi_{\alpha;\beta} = \phi_{\alpha,\beta} - \Gamma^\mu_{\alpha\beta}\phi_\mu \tag{3}$$

BALANCE EQUATIONS

The mechanical balance equations for the surface densities (quantities per unit area) are [2]:

Balance of mass:

$$\frac{\partial}{\partial t}(\rho_s) - 2\rho_s K_M w_\perp + (\rho_s w^\alpha)_{;\alpha} = -[\![\rho(v^m - w^m)]\!]e_m \quad . \tag{4}$$

$\underline{w}$ is the velocity mapping the surface from an initial position to a later one with component $w_\perp$ normal to the surface.(ρ_s: surface mass density, $\underline{v}$: material velocity in the bulk.) Note that all vectors and tensors have also components perpendicular to the surface.

Balance of momentum:

$$\begin{aligned}\frac{\partial}{\partial t}(\rho_s w^k) - 2\rho_s w^k K_M w_\perp + (\rho_s w^k w^\alpha - t_s^{k\alpha})_{;\alpha} &= \\ = [\![- t^{km} + \rho v^k(v^m - w^m)]\!]e_m + \rho_s g^k &\quad .\end{aligned} \tag{5}$$

($\underline{\underline{t}}_s$: surface stress tensor,$\underline{\underline{t}}$: stress tensor defined in the bulk, $\underline{g}$: acceleration of external fields).

Balance of spin:

$$\begin{aligned}&\frac{\partial}{\partial t}(\rho_s s_s^k) - 2K_M w_\perp \rho_s s_s^k + (s_s^k w^\alpha - \Pi_s^{k\alpha})_{;\alpha} \\ &= [\![\Pi^{km} - \rho s^k(v^m - w^m)]\!]e_m + \rho_s m_s^k + \varepsilon^k_{\ lm}\tau^l_\alpha t_s^{m\alpha}\end{aligned} \tag{6}$$

($\underline{s}_s$: spin density defined on the surface, $\underline{\underline{\Pi}}_s$: surface couple stress tensor, $\underline{m}_s$: surface couple forces, $\underline{s}$: spin density in the bulk, $\underline{\underline{\Pi}}$: couple stress tenso).r

Balance of internal energy:

$$\begin{aligned}
\frac{\partial}{\partial t}(e_s\rho_s) - 2K_M w_\perp \rho_s e_s + q^\alpha_{s;\alpha} - w_{s\beta;a} \quad t^{\beta\alpha}_s - \frac{1}{\theta}s_{s\beta;\alpha}\Pi^{\beta\alpha}_s + (\rho_s e_s w^\alpha)_{;\alpha} =& \\
= \quad -[q^m - (v_k - w_k)t^{km} + (\frac{1}{\theta}s_k - \frac{1}{\theta}s_{sk})\Pi^{km} + \rho e(v^m - w^m) +& \\
+ \quad \frac{\rho}{2}(v^k - w^k)(v^k - w^k)(v^m - w^m) + \frac{\rho}{2\theta}(s^k - s^k_s)(s^k - s^k_s)(v^m - w^m)]e_m +& \\
+ \quad \rho_s r_s - \varepsilon^k{}_{lm}\tau^l_\alpha t^{m\alpha}_s \frac{1}{\theta}s_{sk}& \qquad (7)
\end{aligned}$$

(e_s: surface internal energy, e: internal energy in the bulk, $\underline{q}_s$: surface heat flux, $\underline{q}$: heat flux, θ: moment of inertia of the particles).

Into all these balances the curvature enters explicitly through the mean curvature K_M and implicitly through the covariant derivative. The balance equations for the surface quantities are coupled to those for the bulk quantities through the jump terms $[\varphi] := \varphi_+ - \varphi_-$, φ_+ and φ_- being the limiting values of the bulk fields on both sides of the surface. The discontinuity of the bulk fields plays the role of an additional production term in the surface balances.

If electromagnetic fields are present, one has to take into account also Maxwell's equations. They are equivalent to a set of conservation equations for the electric charge and the magnetic flux:

$$\begin{aligned}
\frac{\partial q^t_s}{\partial t} - 2q^t_s K_M w_\perp + (q^t_s w^\alpha + J^{t\alpha}_s)_{;\alpha} &= \\
= \quad -[q^t(v^m - w^m) + J^{tm}]e_m& \\
\underline{e} \times [\underline{E}] - w_\perp[\underline{B}] = 0 \quad .& \qquad (8)
\end{aligned}$$

Here q^t_s is the sum of the free electric charge ρ^e and the polarisation charge, both defned on the surface

$$q^t_s = \rho^e_s - \nabla \cdot \underline{P}_s \quad , \qquad (9)$$

and

$$\underline{J}^t_s := \underline{J}_s + \frac{\partial \underline{P}_s}{\partial t} + 1/\mu_0 \nabla \times \underline{M} \qquad (10)$$

($\underline{J}_s$: current of free electric charges on the surface, $\underline{P}_s$: surface polarisation density).

The mechanical balance equations and Maxwell's equations are the equations of motion for the fields of surface mass density, surface temperature, surface momentum, surface spin, electric field and magnetic induction. The constitutive equations necessary to close the system of differential equations wil be discussed in the fourth chapter.

The geometry of the surface is determined by the geometry at an initial time and the mapping velocity $\underline{w}$. In this sense the balance of surface momentum is the equation of motion for the surface geometry.

EQUATION OF MOTION FOR THE ALIGNMENT

The orientational ordering in a liquid crystal is described by an orientational distribution function (ODF) assigned to each volume element [3], [4]. The first anisotropic moment of this ODF is the alignment tensor of second order $\underline{\underline{a}}$. This is assumed to be the only relevant variable for the orientational ordering. Higher order alignment tensors are not taken into account. The alignment tensor does not enter explicitly the mechanical and electromagnetic balance equations. Therefore an additional equation of motion for this quantity is needed. This equation of motion can be derived from a mesoscopic theory [3], where all field quantities depend not only on position and time, but also on the orientation of the molecule. The mesoscopic surface balance of mass for two dimensional systems reads:

$$\frac{\partial}{\partial t}(\tilde{\rho}_s) - 2\tilde{\rho}_s K_M w_\perp + (\tilde{\rho}_s w^\alpha)_{;\alpha} + \nabla_n \cdot (\underline{u}\tilde{\rho}_s) \quad = \quad -[\![\tilde{\rho}(\tilde{v}^m - w^m)\overset{\cdot}{]\!]}e_m \qquad (11)$$

($\tilde{\rho}_s$: mesoscopic surface mass density, $\underline{u}$: orientational change velocity, $\underline{\tilde{v}}$: mesoscopic material velocity).

The ODF is given by the fraction of particles of orientation $\underline{n}$ over the whole surface density of mass:

$$f_s^{ODF} := \frac{\tilde{\rho}_s(\underline{x}_s, \underline{n}, t)}{\rho_s(\underline{x}_s, t)} \quad . \qquad (12)$$

With this definition of the ODF the mesoscopic surface mass balance is an equation of motion for the ODF defined on the surface:

$$\begin{aligned}
&\frac{\partial}{\partial t} f_s^{ODF} + 1/\rho_s \frac{\partial \rho_s}{\partial t} f s^{ODF} + \\
+ \quad &(f_s^{ODF} w^\alpha)_{;\alpha} + (\rho_{s;\alpha}/\rho_s) f_s^{ODF} w^\alpha + \nabla_n \cdot (\underline{u} f_s^{ODF}) - \\
- \quad &2K_M w_\perp f_s^{ODF} = [\![\tilde{\rho}(\hat{v}^m - w^m)]\!] e^m \quad . \qquad (13)
\end{aligned}$$

Analogously to the three dimensional case [4] one can obtain a system of equations of motion for the alignment tensors of successive order by taking moments of this equation. The only relevant equation here is that for the second order alignment tensor. In addition we make the assumptions that the film is impermeable, i. e. that there is no material flux through the film and that the translational velocity does not depend on the orientation. The resulting equation of motion is:

$$\begin{aligned}
\frac{da_{mn}}{dt} - 2K_M w_\perp a_{mn} - 2 \quad & \overline{(\underline{\omega} \times \underline{\underline{a}})}_{mn} = \\
= \quad & 5/8\pi \left(\sum_{l\,even} (2l-1)!![\oint_{S^2} \overline{n_{k1} \ldots n_{kl}}\; \overline{n_m n_n}\; (\nabla_n \times (\underline{n} \times \underline{u})) \cdot d^2n \right) a^{(l)}_{k1 \ldots kl} + \\
+ \quad & \oint_{S^2} \overline{n_m n_n}\; \left(\nabla_n \times (\underline{n} \times \underline{u})) \cdot d^2n \right) := \underline{\underline{G}} \quad . \qquad (14)
\end{aligned}$$

$a^{(l)}$ are higher order alignment tensors, and $\overline{\quad}$ denotes the symmetric irreducible part of a tensor. The right hand side is the alignment production, a constitutive quantity.

CONSTITUTIVE EQUATIONS

To get a closed system of differential equations for $\rho_s, T_s, \underline{w}$ (or the geometry respectively), $\underline{s}_s, \underline{\underline{a}}, \underline{E}$, and $\underline{B}$ out of the mechanical balances (4) - (7), Maxwell's equations (8) and the alignment tensor balance (14) one needs constitutive equations for $\underline{\underline{t}}_s, \underline{\underline{\Pi}}_s, \underline{m}_s, e_s, \underline{q}_s, q^t_s, \underline{J}_s$ and the alignment production $\underline{\underline{G}}$. One also needs constitutive equations for the jump terms $[\cdots]$, but these will not be considered in the following. For the constitutive mappings the domain has to be fixed, i. e. the state space has to be chosen. A reasonable choice of the set of relevant variables for our problem is

$$\begin{aligned}
\mathrm{Z} \quad = \quad & \{\rho_s, T_s, \rho_{s,\alpha}, T_{s,\alpha}, a^{kl}_s, a^{kl}_{s,\alpha}, a^{kl}_{s,\alpha\beta}, \\
& e^k, e^k_{,\alpha}, \tau^k_\alpha, \tau^k_{\alpha,\beta}, \Gamma^\mu_{\alpha\beta}, E^k, B^k, E^k_{,\alpha}, B^k_{,\alpha}\} \quad . \qquad (15)
\end{aligned}$$

In addition to the fundamental fields and gradients of these the normal to the surface $\underline{e}$, a basis for the tangential space $\underline{\tau}^1, \underline{\tau}^2$, their gradients and the Christoffel symbols Γ are included to take into account the geometry of the surface. It has been assumed that the constitutive surface quantities depend only on the surface fields. Of course this assumption cannot be made for the jump contributions.

The state space (15) is suitable for calculations because it includes partial derivatives and no covariant derivatives, for which no chain rule applies. The covariant derivatives can be constructed from the variables (15) as the Christoffel symbols are included. The constitutive quantities should depend only on covariant derivatives and on intrinsic quantities characterizing the surface geometry. Such intrinsic quantities are the metric $\underline{\underline{g}}$, the curvature tensor (the second fundamental form) $\underline{\underline{b}}$ and the following invariants up to second order in $\tau^k_{\alpha,\beta}$ and $e^k_{,\alpha}$:

$$I^0 \quad = \quad \tau^k_{\gamma;\delta} \tau^{k\gamma;\delta} \qquad (16)$$

$$I^1 = \tau^{k\,\gamma}_{\gamma;}\tau^{k\,\delta}_{\delta;} \tag{17}$$

$$I^2 = \tau^{k}_{\gamma;\delta}\tau^{k}_{\epsilon}\tau^{l\gamma;\epsilon}\tau^{l\delta} \tag{18}$$

$$I^3 = \tau^{l}_{\gamma;\delta}\tau^{l}_{\epsilon}\tau^{k\epsilon;\gamma}\tau^{k\delta} \tag{19}$$

The set of variables (15) does not include the spin and the velocity gradient. Therefore flow cannot be described here, but this may be less important for free standing films.

The Second Law of Thermodynamics implies restrictions on the constitutive mappings. These can be derived from the dissipation inequality

$$\frac{\partial}{\partial t}(\rho_s\eta_s) - 2\rho_s\eta_s K_M w_\perp + (\rho_s\eta_s w^\alpha + \varphi_s^\alpha)_{;\alpha} = -[\rho\eta(v^m - w^m) + \varphi^m]e_m \geq 0 \tag{20}$$

with the balance equtions (4) - (14) as constraints [5], [6].

RESULTS FROM THE SECOND LAW

The surface free energy is defined as $f_s = e_s - T_s\eta_s$. The dissipation inequality implies the following relations:

$$\frac{\partial f_s}{\partial u_A} - \frac{\partial q_s^t}{\partial u_A}\left(\frac{\partial q_s^t}{\partial T_s}\right)^{-1}\left(\frac{\partial fs}{\partial T_s} - \eta_s\right) = 0 \tag{21}$$

for

$$u_A \in \{\rho_{s,\alpha}, T_{s,\alpha}, a^{kl}_{s,\alpha\beta}, E^k_{,\alpha}, B^k_{,\alpha}\} \quad . \tag{22}$$

Therefore, the free energy does not depend on the following derivatives, if no surface charges are present:

$$\frac{\partial f_s}{\partial u_A} = 0 \quad \text{for} \quad u_A \in \{\rho_{s,\alpha}, T_{s,\alpha}, a^{kl}_{s,\alpha\beta}, E^k_{,\alpha}, B^k_{,\alpha}\} \quad . \tag{23}$$

The surface stress tensor is completely determined by the restrictions the Second Law imposes. It's symmetric part is:

$$t_s^{(\alpha\beta)} = \rho_s^2 g^{\alpha\beta}\left[\left(\frac{\partial q_s^t}{\partial T_s}\right)^{-1}\left(\frac{\partial fs}{\partial T_s} - \eta_s\right)\frac{\partial q_s}{\partial \rho_s} - \left(\frac{\partial f_s}{\partial \rho_s}\right)\right] \quad . \tag{24}$$

This part is isotropic like for a simple fluid, because the velocity gradient is not taken into account here. The part describing the stress in a shear experiment is of course anisotropic. The total charge density (the sum of the free charge density and the polarisation charge density) gives an additional contribution to the stress tensor.

For phase boundaries of simple fluids it is often assumed (see for instance [1]) that the normal stresses vanish, i. e. that a force applied tangential to the surface results in a stress vector being also tangential to the surface. For phase boundaries between liquid crystalline phases, thin films, and so on the normal stresses do not vanish. They have been calculated from the dissipation inequality as

$$\begin{aligned}
t_s^{\perp\beta} &= -\rho_s\frac{\partial f_s}{\partial e^k}\tau^k_\delta g^{\delta\beta}+\rho_s\frac{\partial f_s}{\partial\tau^k_\beta}e^k-\rho_s\frac{\partial f_s}{\partial e^k_{,\alpha}}\Gamma^\nu_{\mu\alpha}g^{\mu\beta}\tau^k_\nu-\\
&- \rho_s\frac{\partial f_s}{\partial e^k_{,\alpha}}b^\beta_\alpha e^k+\rho_s\frac{\partial f_s}{\partial\tau^k_{\beta,\mu}}e^k_{,\mu}-\rho_s\frac{\partial f_s}{\partial\tau^k_{\alpha,\beta}}b^\gamma_\alpha\tau^k_\gamma+\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}\rho_s\eta_s\Big(-\frac{\partial q^t_s}{\partial e^k}\tau^{k\beta}+\\
&+ \frac{\partial q^t_s}{\partial\tau^k_\beta}e^k-\frac{\partial q^t_s}{\partial e^k_{,\alpha}}\Gamma^\nu_{\mu\alpha}g^{\mu\beta}\tau^k_\nu-\frac{\partial q^t_s}{\partial e^k_{,\alpha}}g^{\mu\beta}b_{\mu\alpha}e^k+\frac{\partial q^t_s}{\partial\tau^k_{\beta,\mu}}e^k_{,\mu}-\\
&- \frac{\partial q^t_s}{\partial\tau^k_{\alpha,\beta}}b^\gamma_\alpha\tau^k_\gamma\Big)-2a_s^{\perp\beta}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\perp\perp}}+\frac{\partial q^t_s}{\partial a_s^{\perp\perp}}\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}(\rho_s\eta_s-\rho_s\frac{\partial f_s}{\partial T_s})\right)+\\
&+ a_s^{\perp\perp}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\perp\beta}}+\frac{\partial q^t_s}{\partial a_s^{\perp\beta}}\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}(\rho_s\eta_s-\rho_s\frac{\partial f_s}{\partial T_s})\right)-\\
&- a_s^{\alpha\beta}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\perp\alpha}}+\frac{\partial q^t_s}{\partial a_s^{\perp\alpha}}\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}(\rho_s\eta_s-\rho_s\frac{\partial f_s}{\partial T_s})\right)+\\
&+ 2a_s^{\perp\alpha}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\alpha\beta}}+\frac{\partial q^t_s}{\partial a_s^{\alpha\beta}}\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}(\rho_s\eta_s-\rho_s\frac{\partial f_s}{\partial T_s})\right) \quad . \qquad (25)
\end{aligned}$$

The normal stresses are nonzero because of the dependence of the constitutive quantities on the alignment tensor and the geometric variables. Again the surface charge density gives a contribution. As the normal stresses enter the spin balance , they couple the spin balance to that of linear momentum.

Up to here the normal and the tangential vectors to the surface and their derivatives are the geometric variables. But the constitutive quantities should not depend on the choice of the coordinate system in R^3, embedding the surface. Therefore they are allowed only to depend on the intrinsic quantities $\underline{\underline{g}}$, $\underline{\underline{b}}$ and I^0, I^1, I^2, I^3. With these variables the normal stresses read:

$$\begin{aligned}
t_s^{\perp\beta} &= -\rho_s\tau^{k\gamma}_{\ \ ,\gamma}\tau^{k\beta}\left[\frac{\partial f_s}{\partial b^\alpha_\alpha}+(\eta_s-\frac{\partial f_s}{\partial T_s})(\frac{\partial q_s}{\partial T_s})^{-1}\frac{\partial q_s}{\partial b^\alpha_\alpha}\right]+\\
&+ 2\rho_s b_{\gamma\delta}\tau^\delta_m\tau^{m\beta;\gamma}\left[\frac{\partial f_s}{\partial I_2}+\frac{\partial f_s}{\partial I_3}+\right.\\
&+ \left.(\eta_s-\frac{\partial f_s}{\partial T_s})\left(\frac{\partial q_s}{\partial T_s}\right)^{-1}\left(\frac{\partial q_s}{\partial I^2}+\frac{\partial q_s}{\partial I^3}\right)\right]+\\
&+ \rho_s\left(e^{k,\beta}\tau^{k\gamma}_{\gamma;}+2b_\nu{}^\beta\tau^{l\nu}\tau^{l\gamma}_{\ \ ;\gamma}-2b^\mu_\mu\tau^{l\beta}\tau^{l\gamma}_{\ \ ;\gamma}+2b^\beta_\nu\tau^{l\nu}\tau^{l\gamma}_{\ \ ;\gamma}\right)*
\end{aligned}$$

$$
\begin{aligned}
* &\quad \left(\frac{\partial f_s}{\partial I^1} + \left(\eta_s - \frac{\partial f_s}{\partial T_s}\right)\left(\frac{\partial q_s}{\partial T_s}\right)^{-1}\frac{\partial q_s}{\partial I^1}\right) \\
+ &\quad 2\rho_s\left(\tau^{k\beta;\mu}e_{k,\mu} + b^{\mu}_{\gamma}\tau^{l\beta}\tau^{l\gamma;\mu}\right)\left(\frac{\partial f_s}{\partial I^0} + \left(\eta_s - \frac{\partial f_s}{\partial T_s}\right)\left(\frac{\partial q_s}{\partial T_s}\right)^{-1}\frac{\partial q_s}{\partial I^0}\right) \\
+ &\quad 2\rho_s\left(b^{\beta\gamma}\tau^{l}_{\gamma}\tau^{l\delta}{}_{;\delta} + b^{\gamma}_{\gamma}\tau^{l\beta}\tau^{l\delta}{}_{;\delta}\right)\left(\frac{\partial f_s}{\partial I^1} + \left(\eta_s - \frac{\partial f_s}{\partial T_s}\right)\left(\frac{\partial q_s}{\partial T_s}\right)^{-1}\frac{\partial q_s}{\partial I^1}\right) \\
- &\quad 2\rho_s\left(-b^{\gamma}_{\alpha}\tau^{k}_{\gamma}\tau^{k\alpha;\beta} + b^{\gamma}_{\alpha}\tau^{l\alpha;\gamma}\tau^{l\beta}\right)\left(\frac{\partial f_s}{\partial I^0} + \left(\eta_s - \frac{\partial f_s}{\partial T_s}\right)\left(\frac{\partial q_s}{\partial T_s}\right)^{-1}\frac{\partial q_s}{\partial I^0}\right) \\
- &\quad 2a_s^{\perp\beta}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\perp\perp}} + \frac{\partial q_s^t}{\partial a_s^{\perp\perp}}\left(\frac{\partial q_s^t}{\partial T_s}\right)^{-1}\left(\rho_s\eta_s - \rho_s\frac{\partial f_s}{\partial T_s}\right)\right) + \\
+ &\quad a_s^{\perp\perp}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\perp\beta}} + \frac{\partial q_s^t}{\partial a_s^{\perp\beta}}\left(\frac{\partial q_s^t}{\partial T_s}\right)^{-1}\left(\rho_s\eta_s - \rho_s\frac{\partial f_s}{\partial T_s}\right)\right) - \\
- &\quad a_s^{\alpha\beta}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\perp\alpha}} + \frac{\partial q_s^t}{\partial a_s^{\perp\alpha}}\left(\frac{\partial q_s^t}{\partial T_s}\right)^{-1}\left(\rho_s\eta_s - \rho_s\frac{\partial f_s}{\partial T_s}\right)\right) + \\
+ &\quad 2a_s^{\perp\alpha}\left(\rho_s\frac{\partial f_s}{\partial a_s^{\alpha\beta}} + \frac{\partial q_s^t}{\partial a_s^{\alpha\beta}}\left(\frac{\partial q_s^t}{\partial T_s}\right)^{-1}\left(\rho_s\eta_s - \rho_s\frac{\partial f_s}{\partial T_s}\right)\right) \quad . \qquad (26)
\end{aligned}
$$

The symmetric part of the stress tensor (24) and the normal stresses (26) depend only on variables not vanishing in equilibrium. Therefore they have the same form in equilibrium as calculated here for nonequilibrium. But in equilibrium the alignment tensor is not an independent variable, but depends on the equilibrium variables ρ_s, T_s and the geometry.

Now one has to use representation theorems [7] to make ansatzes for the surface free energy density and the charge density. The constraints (23) have to be taken into account. As one gets then very long expressions involving many phenomenological constants they are omitted here.

The exploitation of the dissipation inequality results in some more restrictions on constitutive functions, for instance

$$
\frac{\partial \varphi_s}{\partial u_A} - \frac{1}{T}\frac{\partial q_s}{\partial u_A} = 0 \qquad (27)
$$

for

$$
u_A \in \{\rho_{s,\alpha}, T_{s,\alpha}, a^{kl}_{s,\alpha\beta}, E^{k}_{,\alpha}, B^{k}_{,\alpha}\} \quad . \qquad (28)
$$

It is often assumed that there are no couple stresses at all. Then the difference between the heat flux devided by the temperature and the entropy flux does not depend on the variables (28) . But the difference does not vanish identically as it is assumed in the classical Irreversible Thermodynamics.

The residual inequality [8] gives the entropy production :

$$\begin{aligned}
\sigma \;=\;& P^{\eta}_{[\;]} + P^{\rho}_{[\;]}\frac{\rho_s}{T_s}\left(\frac{\partial f_s}{\partial \rho_s} + \left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}\left(\eta_s - \frac{\partial f_s}{\partial T_s}\right)\right) - \\
-\;& \frac{1}{T_s}P^{e}_{[\;]} - \frac{\rho_s}{T_s}\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}\left(\eta_s - \frac{\partial f_s}{\partial T_s}\right)J^{t\alpha}_{s\;;\alpha} - \frac{\rho_s}{T_s}\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}\left(\eta_s - \frac{\partial f_s}{\partial T_s}\right)P^{q}_{[\;]} + \\
+\;& \left(P^{\underline{\underline{a}}kl}_{[\;]} - G^{kl}\right)\left(\frac{\rho_s}{T_s}\frac{\partial f_s}{\partial a^{kl}_s} - \frac{\partial q^t_s}{\partial a^{kl}_s}\frac{\rho_s}{T_s}\left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}\left(-\eta_s + \frac{\partial f_s}{\partial T_s}\right)\right) - \\
-\;& \frac{1}{T^2_s}q^{\alpha}_s T_{s,\alpha} \geq 0 \qquad (29)
\end{aligned}$$

with the jump contributions

$$\begin{aligned}
P^{\eta}_{[\;]} \;:=\;& [\rho(\eta - \eta_s)(v^m - w^m)]e_m \\
P^{\rho}_{[\;]} \;:=\;& [\rho(v^m - w^m)]e_m \\
P^{e}_{[\;]} \;:=\;& [\rho(e - e_s)(v^m - w^m) + q^m - (v_k - w_k)t^{km} - 1/\theta(s_k - s_{sk})\Pi^{km} + \\
+\;& 1/2\rho(v^k - w^k)^2(v^m - w^m) + \frac{1}{2\theta}\rho(s^k - s^k_s)^2(v^m - w^m)]e_m \\
P^{q}_{[\;]} \;:=\;& \left(\frac{\partial q^t_s}{\partial T_s}\right)^{-1}\left(-\eta_s + \frac{\partial f_s}{\partial T_s}\right)[\rho q^t(v^m - w^m) + J^{tm}]e_m \\
P^{\underline{\underline{a}}kl}_{[\;]} \;:=\;& [\rho a^{kl}(v^m - w^m)]e_m \quad . \qquad (30)
\end{aligned}$$

EQUILIBRIUM CONDITIONS

Equilibrium states are stationary states with vanishing fluxes. If the jump terms (30) in the entropy production vanish also in nonequilibrium, the entropy production is a sum of fluxes and forces, as it is assumed in the classical Thermodynamics of Irriversible Processes. Then (and only then) it can be concluded [9] that in equilibrium

$$T_{s,\alpha} = 0 \qquad \frac{\partial f_s}{\partial T_s} = \eta_s \quad . \qquad (31)$$

These are the same equilibrium conditions one has in three dimensions.

Analogously to liquid crystals in three dimensions [10] a variational principle for two dimensional liquid crystals can be derived [11]. The total surface free energy is extremal in equilibrium. The corresponding Euler-Lagrange equations

$$\frac{\partial f_s}{\partial T_s} - \nabla_\alpha \frac{\partial f_s}{\partial T_{s,\alpha}} = 0 \tag{32}$$

$$\frac{\partial f_s}{\partial \rho_s} - \nabla_\alpha \frac{\partial f_s}{\partial \rho_{s,\alpha}} = 0 \tag{33}$$

$$\frac{\partial f_s}{\partial a_s^{kl}} - \nabla_\alpha \frac{\partial f_s}{\partial a_{s,\alpha}^{kl}} + \nabla_\alpha \nabla_\beta \frac{\partial f_s}{\partial a_{s,\alpha\beta}^{kl}} = 0 \tag{34}$$

result with (23) in

$$\begin{aligned} \frac{\partial f_s}{\partial T_s} &= 0 \\ \frac{\partial f_s}{\partial \rho_s} &= 0 \\ \frac{\partial f_s}{\partial a_s^{kl}} - \nabla_\alpha \frac{\partial f_s}{\partial a_{s,\alpha}^{kl}} &= 0 \end{aligned} \tag{35}$$

in equilibrium and in the absence of surface charges. With a representation theorem for the free energy (35) determines the alignment tensor field.

The surface geometry has to be calculated from the balance of momentum in equilibrium

$$t_s^{k\alpha}{}_{;\alpha} = \rho_s g^k \tag{36}$$

with the stress tensor (24) and (26).

In the following last chapter electromagnetic fields will not be taken into account.

OUTLOOK: ALIGNMENT PRODUCTION

The Second Law of Thermodynamics does not imply any restrictions on the alignment production $\underline{\underline{G}}$, and a purely phenomenological theory cannot get a closed differential equation for the second order alignment tensor out of equation (14). As can be seen from (14) the alignment production is determined by the higher order alignment tensors $a^{(l)}$ and the orientational change velocity $\underline{u}$. A way leading to these quantities [12] starts from a statistical description on the phase space Γ. The phase space is spanned by the positions of the particles $\underline{x}_1 \cdots \underline{x}_N$, their orientations $\underline{n}_1 \cdots \underline{n}_N$ and the respective velocities $\dot{\underline{x}}_1 \cdots \dot{\underline{x}}_N$, $\dot{\underline{n}}_1 \cdots \dot{\underline{n}}_N$ with $\{\underline{x}_1 \cdots \underline{x}_N\} \in \mathbb{R}^3$, $\{\underline{n}_1 \cdots \underline{n}_N\} \in S^2$, $\{\dot{\underline{x}}_1 \cdots \dot{\underline{x}}_N\} \in \mathbb{R}^3$ and $\{\dot{\underline{n}}_1 \cdots \dot{\underline{n}}_N\} \in TS^2$. $\bar{\Gamma}$ denotes the coordinates in Γ-space. For the fields of mass density, energy, momentum, spin and alignment tensor corresponding Γ-space observables are introduced like

$$\begin{aligned}\hat{\rho}(\bar{\Gamma};\underline{x}) &= \sum_{\alpha=1}^{N}\delta(\underline{x}-\underline{x}^{\alpha})\\ \hat{\underline{\underline{a}}}(\bar{\Gamma};\underline{x}) &= \sum_{\alpha=1}^{N}\overline{\underline{n}^{\alpha}\underline{n}^{\alpha}}\;\delta(\underline{x}-\underline{x}^{\alpha})\end{aligned}\tag{37}$$

and similiarly for the higher order alignment tensors. N is the total number of particles, $\underline{x}^{\alpha}$ the position of particle α and $\underline{n}^{\alpha}$ the orientation of particle α. Note that these observables depend on the Γ-space coordinates and on the position $\underline{x}$ in the continuum. The phase space distribution function is supposed to give the averages for the fields of mass, energy, momentum, spin and second order alignment tensor correctly. Beside these constraints it is determined such as to maximize the entropy $\int_{\Gamma} f^{phasespace}(\bar{\Gamma})\ln f^{phasespace}(\bar{\Gamma})d\bar{\Gamma}$ [13]. With this phase space distribution function all the higher order alignment tensors can be calculated:

$$a^{(k)}(\underline{x},t) = \int_{\Gamma}\sum_{\alpha=1}^{N}\overline{\underline{n}_1^{\alpha}\cdots\underline{n}_k^{\alpha}}\;\delta(\underline{x}-\underline{x}^{\alpha})f^{phasespace}(\bar{\Gamma},t)d\bar{\Gamma} \quad .\tag{38}$$

For the alignment production one also needs the orientational change velocity $\underline{u}$. This will be dicussed in future publication.

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