Lagrangian field theory of plasticity and dislocation dynamics
Attempts towards unification with thermodynamics of irreversible processes (*)

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

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WITHIN THE LAGRANGE FORMALISM, a mechanical continuum theory of disloca-
tion dynamics is presented, which results in a phenomenological, unified descrip-
tion of elastic and plastic deformations of a crystal. Further developments towards
a thermo-mechanical theory including dissipation are methodically envisaged. The
theory is based on complex matter fields and vortex potentials as fundamental field
variables. Especially the dislocation network is divided into different classes of equal
dislocations, giving rise to a more refined description of the dislocation dynamics as
traditionally can be done by the well-known dislocation density tensor. Each class
of dislocations is associated with a complex dislocation field. The elastic interaction
between dislocations of different classes results in correlational effects which cannot
be described by means of the traditional continuum theory of dislocations. Whereas
in traditional approaches the plastically deforming body is formally looked upon as
an elastic solid with inherent flow properties, we are looking at such a system in
a reverse manner: The plastically deforming body is formally regarded as a fluid
with inherent solid properties. Formally the plastically deforming body is associated
with a generalized Cosserat fluid based on matter and dislocation fields. In this way
we overcome the difficulties due to the deformation chaos produced by dislocation
motion.

1. The aim

WITHIN THE FRAMEWORK of Lagrange formalism (LF) we aim at a phenomeno-
logical plasticity theory based on dislocation dynamics. The theory is intended
as a *methodical unification of elasticity and plasticity*. It will be a dynamical
generalization of the well-established eigenstress theory of dislocations. Plastic-
ity being extremely dissipative we finally intend to include thermodynamics of
irreversible processes (TIP) along the unifying procedure of LF. With regard to

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(*) Conventions: Tensors are marked by bold-type symbols. If not stated otherwise, indices
occurring twice in a product imply summation over the range of the index.

TIP the theory of plasticity will be formulated in quite a different manner as compared with traditional attempts.

Roughly speaking, the whole information on static elasticity of a deformable body is contained in an elastic potential $W(\nabla\vec{u}) = W(\mathbf{e})$, W being the density of elastic energy, $\vec{u}$ the elastic displacement field and $\mathbf{e}$ the associated strain tensor. The function W is the kernel of the elastic energy functional U, which in statics defines the fundamental variational principle of minimal energy:

$$(1.1) \qquad U = \int_V W \, dV = \text{minimum},$$

by free variation of $\vec{u}$.

The associated Euler–Lagrange equations (ELEqs.),

$$(1.2) \qquad \nabla\cdot\boldsymbol{\sigma} = 0,$$

are the equilibrium conditions, i.e. the fundamental dynamical equations in the case of statics.

$$(1.3) \qquad \boldsymbol{\sigma} = \frac{\partial W}{\partial \mathbf{e}}$$

defines the constitutive equations for the stress tensor $\boldsymbol{\sigma}$.

The dynamical generalization of Eq. (1.1) is *Hamilton's variational principle*:

$$(1.4) \qquad J = \int_{t_1}^{t_2}\int_V l(\vec{u}, \partial_t\vec{u}, \nabla\vec{u}) \, dV \, dt = \text{extremum},$$

by free variation of $\vec{u}$.

Now the total information on the processes is involved in the Lagrangian l. The ELEqs. as the fundamental field equations are the *equations of motion*:

$$(1.5) \qquad \partial_t\frac{\partial l}{\partial(\partial_t\vec{u})} + \nabla\cdot\frac{\partial l}{\partial(\nabla\vec{u})} - \frac{\partial l}{\partial\vec{u}} = 0 \,.$$

Obviously, there are two remarkable features involved in the theory: There are *universal structures* (Eqs. (1.1)–(1.5)), which apply in the same way to all elastic materials, whereas the particular forms of the functions $W(\mathbf{e})$ and $l(\ldots)$ are *individual structures*, which depend on the particular material. They have to be fitted to experimental data (elastic moduli)[1].

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[1] It should be mentioned that the frequently used formula "kinetic minus potential (elastic) energy" for l is but a dogma, which belongs to the individual structures insofar, as it only approximately describes the dynamics of an elastically deformed body. An exact Lagrangian for this case will be given in this paper, too.

We aim at a generalization of this unifying procedure in such a way as to imply the dynamics of plasticity. From the very beginning this theory will be based on dislocation dynamics. In this paper we shall confine our considerations to pure mechanics, adding perspectives for the inclusion of TIP. Single crystals are the systems we have in mind. Dissipation, which is a main feature of plasticity, will be involved in a future step.

2. The physical situation – fundamental ideas

2.1. Deformation chaos

On the microscale, the phenomenological plasticity is based on dislocation dynamics. *Dislocation motion*, however, *is associated with deformation chaos* [1]. The situation is demonstrated by means of the cartoon in Fig. 1:
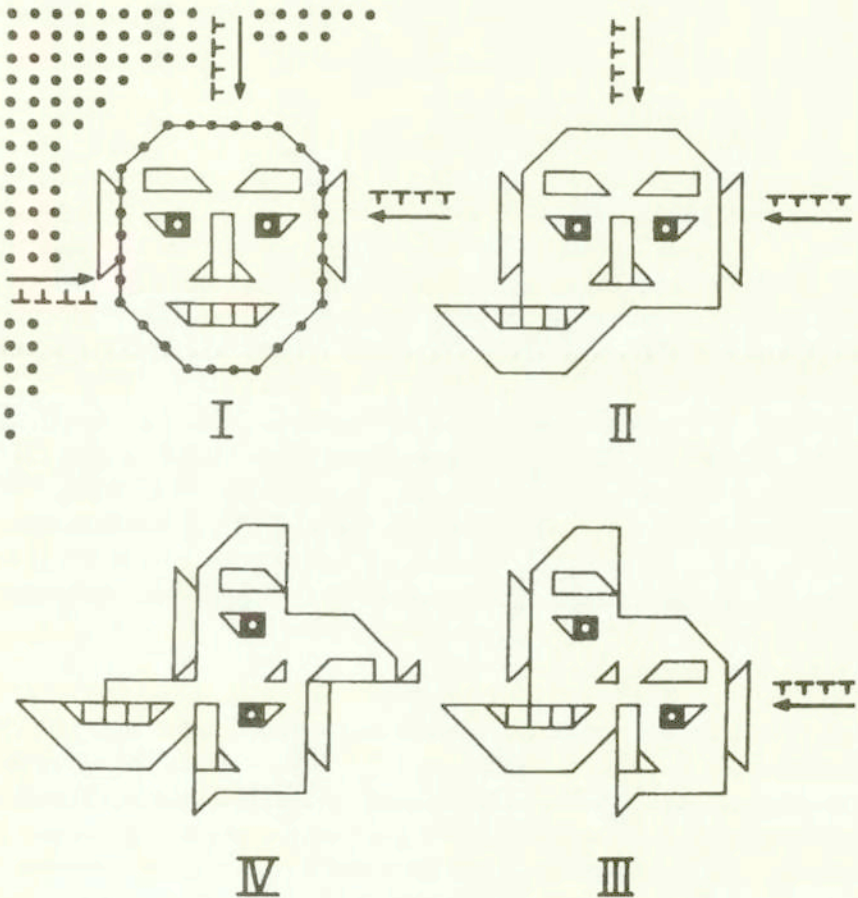

FIG. 1. Deformation chaos due to dislocation motion.

One after the other, three dislocation cascades are running through the crystal. The crystal lattice remains almost perfect except for the actual sites of the dislocations. Nevertheless the crystal gets chaotically torn; material neighbourhoods get completely destroyed. The scales relevant for this chaos are given by the relevant scales of the dislocation network, i.e. by the distances of the active glide planes and by the lengths of the running dislocation cascades. This means, however, that the relevant scales reach from micro to macro-dimensions. In this context one should keep in mind the sliplines and Lüders-bands which can be seen on the surface of a plastically torn specimen nearly with naked eyes.

As a consequence of this situation the traditional concepts for the deformation of solids have to be left. Neither a displacement field nor a material coordinate system dragged along with a deformation makes physical sense; *the plastically deformed body is not a material manifold!*

■ We look at the plastically deforming body by means of *mass densities* and *fluxes*. That's the point of view of TIP, which will be a guide-line throughout our whole approach. Within Lagrange formalism this sight will be realized by means of complex *matter fields*. ■

2.2. Correlational effects

Traditional dislocation theory is based on the *dislocation density* tensor α which geometrically is associated with torsion of the dislocated crystal lattice. This tensor, however, is locally but an averaged measure of the dislocation arrangement. It might vanish even though a vivid dynamics of dislocations of opposite signs takes place in plasticity. So, correlational effects, kinematical as well as dynamical ones, have to be taken into account in plasticity by means of non-traditional tools.

■ We look at dislocation dynamics in a more refined way by dividing the dislocation network into different *classes of equal dislocations* [1, 2, 3, 22]. Within LF each class will be associated with a *complex dislocation field*. Along this line we are particularly able to introduce into LF the interactions between dislocations of different types; we thus take account of correlations within the dislocation network. For realistic plasticity problems only a few classes are really relevant. ■

2.3. Thermodynamics and plasticity

The dislocation network is *far away from thermal equilibrium*. The energy of a dislocation per atomic unit length is 1 ... 10 eV, whereas the thermal energy at room temperature is $kT \sim 1/20$ eV. Dislocation dynamics is extremely dissipative, even at a very low plastic deformation rate. As a consequence there is *no reversible plastic deformation process*, i.e. there is *no thermostatics of plasticity available* which could be extrapolated into the regime of non-equilibrium thermodynamics, e.g. along the line of Onsager's approach to TIP [4].

■ Lagrange formalism allows for any dynamics, even far away from equilibrium. So, especially with regard to thermal effects, we describe dislocation dynamics and plasticity within the framework of LF [1, 2, 3, 22].

It has been shown that TIP can be involved in LF, too [5, 6, 7]. As an essential feature of this theory each degree of freedom, which gives rise to entropy production, has to be represented by a complex field variable. Especially this holds for disipative degrees of freedom. The entropy concept, which is involved in the theory in a natural and straightforward way, is associated with the invariance of the Lagrangian with respect to a common gauge transformation of all complex field variables [8]. As a methodical consequence, all dissipative processes have to be described by means of complex field variables. This is the reason for introducting complex matter and dislocation fields into our approach to plasticity, as has been mentioned above.

LF as applied to TIP is based on the most fundamental, *complex field of thermal excitation* or the *thermion field*(²) ψ. Dissipation of mechanical energy during plastic deformation will be modelled in LF as an irreversible energy transfer from mechanical degrees of freedom, i.e. from matter and dislocation fields, to thermal degrees of freedom, i.e. to the thermion field [22]. ■

2.4. Creation and annihilation processes in plasticity

There are essentially three regions in the stress-strain curve of a plastically deformed body [11, 12]: Increasing the external load of a body, the initial elastic region is followed by an extended region of plastic softening which finally is followed by a region of plastic hardening. The dynamics of dislocations, i.e. dislocation motion, dislocation reactions, creation and annihilation of dislocations, pinning and depinning of dislocations, are responsible with different relevance for the various regions. Especially the plastic softening is related to a dramatic increase of dislocations due to the activities of Frank — Read sources. Except for the motion of dislocations, all these elementary processes can be looked upon as creation and annihilation processes of mobile and immobile dislocations. They are essentially dissipative.

■ In LF the various *elementary processes of dislocation dynamics will be modelled* step by step by an *appropriate coupling of the various fundamental fields in the Lagrangian.*

With regard to motion, creation and annihilation there are *close analogies between the dynamics of dislocations and ordinary chemical reactions* [13]. The latter ones have already been successfully involved into LF by means of complex matter fields associated with the chemically reacting species [7]. They are physically related with point-like objects like atoms or molecules. Dislocations, however, are line-shaped objects. We take account of this peculiarity by means of the geometrical concept of torsion in a *generalized Cosserat-continuum* [1, 2,

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(²) This nomenclature is due to the quantization of the thermal excitation field [9, 10].

3, 14, 22], whereas the complex dislocation fields associated with different dislocation classes are directly analogous to the matter fields of chemical species. ■

2.5. Stability theory and dislocation dynamics

It is quite evident that *stability and instability* are *inherent features of dislocation dynamics*. We refer *stat. class* pinning and depinning of dislocations and *to* *n* *threshold* of Frank–Read sources. So, the modelling of plastic behaviour has to take into account stability considerations from the very beginning.

■ *In LF there is involved a stability theory in the sense of Lyapunov's direct method* [8]. This holds in a particular manner in the case of TIP based on complex fundamental field variables. A Lyapunov functional can be established from the Lagrangian in an easy and straightforward manner. This structure will play an important role in our future efforts to model plasticity. ■

Summing up the preceding arguments one can say, that Lagrange formalism is an appropriate tool to describe plasticity from the mechanical as well as from the thermodynamical point of view. Looking further at elasticity, which in the past has more or less successfully been established with LF, a methodically unified description of both deformation modes, the elastic and the plastic one, is a most attractive feature of LF.

3. Design of the theory – formal ingredients ([3])

3.1. The Cosserat-fluid as a model for plasticity

Traditionally a plastically deforming crystal has *formally* been looked upon as an elastic solid with particular (plastic) flow properties. We adopt an alternative view: *A plastically deforming crystal will formally be looked upon as a fluid with particular solid (elastic) properties!* In this way we avoid the concept of a material manifold ([4]) from the very beginning, i.e. we get rid of the difficulties associated with the deformation chaos of a plastically deformed body. One should keep in mind, that the deformation of a solid may equally well be looked upon as a material flow!

THE MODEL:

Formally we introduce the concept of a *generalized Cosserat fluid* [2, 3, 14, 22]. This is the quintessence of a *flowing, material carrier*, the elements (mass points) of which are endowed with an *internal structure in the form of deformable triads of Cosserat directors. The flow of the carrier is physically associated with the phenomenological material flow of the deforming crystal*, whereas the *directors*

([3]) The subsequent Subsecs. 3.1–3.3 refer to the Subsecs. 2.1–2.3, respectively.

([4]) In the usual mathematical sense, of course!

are physically associated with the elementary lattice vectors of the crystal. The elastic response of the crystal is locally modelled by the deformation status of the director triad. In a generalized Cosserat-continuum [14] *the deformations of the material carrier and of the director triads are in principle independent.* However, with regard to plasticity of a crystal and depending on the actual deformation modus of the crystal, *there will be particular kinematical couplings between the flow of the material carrier and the deformation of the director triads.* Especially *in the case of dislocation motion,* i.e. of plastic deformation of the crystal, *the dislocation fields will be involved in these kinematical couplings.* It is evident, that this concept takes account of elastic and of plastic deformation simultaneously and in a methodically unified way.

All relevant physical structures of the crystal are embedded in the material carrier. In the case of plasticity this will happen with the dislocation fields, and – taking account of thermo-mechanical effects (dissipation) – it will happen with the thermion field, too, etc.

The *material carrier* is formally described by means of a *complex matter field* Ψ and a *complex vortex potential* Ω as fundamental field variables:

(3.1) $$\Psi(x,t) = \sqrt{\varrho(x,t)} \, \exp(i\Phi(x,t)),$$

(3.2) $$\Omega(x,t) = \sqrt{\Lambda(x,t)} \, \exp(iM(x,t)).$$

They give rise to the definition of the *mass density*

(3.3) $$\varrho(x,t) = \Psi^*(x,t)\Psi(x,t) \geq 0,$$

of the *flow velocity*

(3.4) $$\vec{v}_{(f)}(x,t) = \nabla\Phi(x,t) + \Lambda(x,t)\nabla M(x,t),$$

and of the *vortex field*

(3.5) $$\vec{\omega}(x,t) = \frac{1}{2}\nabla \times \vec{v}_{(f)}(x,t) = \frac{1}{2}\nabla\Lambda(x,t) \times \nabla M(x,t)$$
$$= \frac{1}{2i}\nabla\Omega^*(x,t) \times \nabla\Omega(x,t)$$

as secondary field variables, all of them being identified with the respective physical quantities of the crystal.

With regard to the Eqs. (3.4) and (3.5), the quantities Φ, Λ and M are known as *Clebsch* or *Monge potentials* [24]. In three dimensions such a Clebsch-ansatz can always be done. However, the three potentials are not unique; they are associated with a non-Lie gauge group ([5]). It can be shown, that by properly

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[5] This group becomes essential with regard to the definition of area-type balance equations [15]. See also the paper of M. Scholle [16].

regauging of the Clebsch potentials, the property

$$(3.6) \qquad \Lambda(x,t) = \Omega^*(x,t)\Omega(x,t) \geq 0$$

can always be assumed. Thus, the definition of the complex vortex potential Ω is justified.

Let $\vec{e}_i$, $i = 1, 2, 3$ be the local base vectors of an external, Cartesian coordinate system x^i. Then the *three Cosserat directors*

$$(3.7) \qquad \vec{a}_\kappa(x,t) = A^i_\kappa(x,t)\vec{e}_i, \qquad \kappa = 1, 2, 3,$$

are another set of fundamental field variables. They are defined by a non-singular component matrix $A^i_\kappa(x,t)$, the inverse matrix of which is $A^\kappa_i(x,t)$:

$$(3.8) \qquad A^i_\kappa A^\lambda_i = \delta^\lambda_\kappa, \qquad A^i_\kappa A^\kappa_j = \delta^i_j.$$

The Cosserat directors give rise to the definition of secondary quantities such as the *elastic strain tensor* [17]

$$(3.9)\,(^6) \quad \mathbf{e}(x,t) = (e_{\kappa\lambda}), \qquad e_{\kappa\lambda} = \frac{1}{2}(\vec{a}_\kappa \cdot \vec{a}_\lambda - \delta_{\kappa\lambda}) = \frac{1}{2}\left(A^i_\kappa A^j_\lambda \delta_{ij} - \delta_{\kappa\lambda}\right),$$

and the *affine director connexion* [18]

$$(3.10) \qquad \Gamma(x,t) = \left(\Gamma_{ij}{}^k\right), \qquad \Gamma_{ij}{}^k = A^k_\mu \partial_i A^\mu_j,$$

which in the Cosserat fluid defines a *director parallelism*. In the associated crystal both quantities are identified with the *elastic lattice strain* and the *lattice parallelism*, respectively. The *torsion* involved in the director parallelism is defined by the *torsion tensor* [17, 18]

$$(3.11) \qquad \mathbf{S} = \left(S_{ij}{}^k\right), \qquad S_{ij}{}^k = \Gamma_{[ij]}{}^k = A^k_\mu \partial_{[i} A^\mu_{j]},$$

which in the crystal lattice is identified with the (traditional) *dislocation density tensor* $\boldsymbol{\alpha}$ [17, 19]:

$$(3.12) \qquad \alpha_{ij}{}^k = S_{ij}{}^k.$$

Obviously the complete traditional deformation concept of an elastically deformed and dislocated crystal has been taken over into the model of the Cosserat fluid. However, using the complex fields Ψ and Ω, the deformation of the material carrier is considered as a flow (Eqs. (3.4), (3.5)). This holds for *elastic and plastic deformations of the crystal*. We thus get rid of the traditional, conceptual

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(^{6}) The Euclidean scalar product is involved.

difficulties associated with the deformation chaos, i.e. *there is no displacement field involved in the theory.*

REMARK. One should keep in mind that the *complex* fields Ψ and Ω fit into the entropy concept of LF as applied to TIP [8]. The dynamics of the directors $\vec{a}_\kappa$, however, gives rise to dissipation too. So, these quantities have finally to be also represented by complex fields. This can be done on the basis of a threefold Clebsch-ansatz

(3.13) ([7]) $$\vec{a}^\kappa = \nabla\varphi^\kappa + \xi^\kappa\nabla\eta^\kappa, \qquad \kappa = 1, 2, 3,$$

with

(3.14) $$\nabla \times \vec{a}^\kappa = \nabla\xi^\kappa \times \nabla\eta^\kappa \neq 0,$$

if the director fields are endowed with torsion, i.e. if dislocations are present in the crystal.

Now we distinguish three deformation modes of the Cosserat fluid:

(I) The compatibly, i.e. elastically deforming crystal containing no dislocations is associated with a Cosserat fluid, the directors of which are completely *substantially dragged along* with the carrier's flow. The Cosserat triads are holonomic [18] and they are deforming holonomically. The reader should imagine a compatibly deforming crystal lattice, the lattice points and lattice vectors of which are identified with the material carrier and the directors of the Cosserat-fluid.

(II) The elastically deforming crystal contains dislocations which are fixed in the crystal lattice. This deformation mode is but *a dynamical generalization of the well-known statical eigenstress problem of dislocations* [19]. It is modelled by a Cosserat-fluid, the directors of which are still substantially dragged along with the carrier's flow. The dislocations are substantially dragged along with the deforming crystal, i.e. with the carrier's flow. Speaking in mathematical terms the director triads are anholonomic; however, they are deforming holonomically.

(III) The plastically deforming crystal is associated with dislocations drifting through the crystal. This deformation mode is modelled by a Cosserat fluid, the director triads of which are anholonomic and which are deforming anholonomically; they are *partially dragged along with the fluid* according to the *drift dislocation flux*, the latter one being exclusively responsible for the plastic flow of the body.

The associated kinematical coupling equations will take into account the matter field Ψ, the vortex potential Ω, the flow field $\vec{v}_{(f)}$, the director fields $\vec{a}_\kappa$, the dislocation density $\boldsymbol{\alpha}$ and its related drift dislocation flux $\mathbf{J}$. These equations will be presented in Sec. 4 ([8]).

([7]) See also M. Scholle: Dissertation [20]. $\vec{a}^\kappa$ are reciprocal vectors associated to $\vec{a}_\kappa$.

([8]) Eqs. (4.8)–(4.11), (4.13)–(4.19).

In the cases (I) or (II, III) we call the *Cosserat fluid a compatible* or *incompatible one*, respectively. In any case the deformation state of the Cosserat triads gives rise to a local elastic response of the deforming body.

3.2. Dislocation classes and complex dislocation fields

The dislocation network is divided into different *classes of equal dislocations* (see Fig. 2), which are characterized by the set of three vectors

$$(3.15) \qquad \{\vec{l}, \vec{b}, \vec{m}, \} = \{\text{line vector of the dislocation lines, Burgers vector,}$$

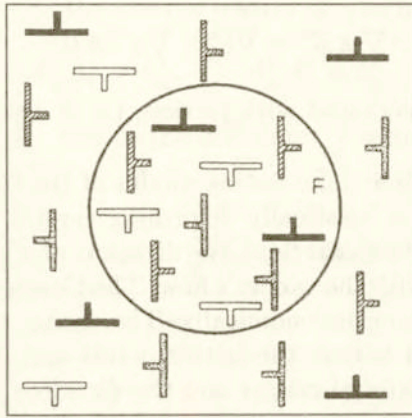$$\text{normal vector of the glide plane}\}.$$

FIG. 2. Different classes of dislocations in the dislocation network.

The dislocations are topologically defined with respect to the crystal lattice: The three vectors are constant with respect to the Cosserat triads, i.e. with respect to the lattice geometry:

$$(3.16) \qquad \vec{l} = l^\kappa \vec{a}_\kappa, \qquad \vec{b} = b^\kappa \vec{a}_\kappa, \qquad \vec{m} = m^\kappa \vec{a}_\kappa,$$

$$\text{all components } l^\kappa, \ b^\kappa, \ m^\kappa = \text{constants.}$$

The line vector $\vec{l}$ is assumed to be a unit vector with respect to the Cosserat triad, i.e. with respect to the lattice geometry; the line vector and the normal vector are by definition perpendicular in the same sense [9]:

$$(3.17) \qquad \vec{l} * \vec{l} = \delta_{\kappa\lambda} l^\kappa l^\lambda = 1, \qquad \vec{l} * \vec{m} = \delta_{\kappa\lambda} l^\kappa m^\lambda = 0.$$

Each class $\{\vec{l}, \vec{b}, \vec{m}\}$ is associated with two complex fields, with a *complex dislocation field*

$$(3.18) \qquad \psi_{\{l,b,m\}}(x,t) = \sqrt{n_{\{l,b,m\}}(x,t)} \exp\left(i\varphi_{\{l,b,m\}}(x,t)\right),$$

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[9] i.e. with respect to the lattice metric $\mathbf{a} = (a_{\kappa\lambda} = \delta_{\kappa\lambda})$: $\quad \vec{u} * \vec{v} = a_{\kappa\lambda} u^\kappa v^\lambda$ [18].

and with a *complex vortex potential*

(3.19)
$$\omega_{\{l,b,m\}}(x,t) = \sqrt{\lambda_{\{l,b,m\}}(x,t)} \exp\left(i\mu_{\{l,b,m\}}(x,t)\right).$$

From these fields we define the *scalar dislocation density within the class* $\{\vec{l}, \vec{b}, \vec{m}\}$,

(3.20)
$$n_{\{...\}}(x,t) = \psi^*_{\{...\}}(x,t)\psi_{\{...\}}(x,t) \geq 0,$$

and the *total dislocation flow velocity of class* $\{\vec{l}, \vec{b}, \vec{m}\}$,

(3.21)
$$\vec{v}_{\{...\}}(x,t) = \nabla\varphi_{\{...\}}(x,t) + \lambda_{\{...\}}(x,t)\nabla\mu_{\{...\}}(x,t).$$

$n_{\{...\}}$ is the *number of dislocations of class* $\{...\}$ *intersecting a unit test area perpendicular to the line direction* $\vec{l}$. It may equally well be interpreted as the *total length of dislocations of class* $\{...\}$ *within a unit volume*, i.e. it is also a good *thermodynamical state variable for the dislocated crystal*. Again we may assume $\lambda_{\{...\}}(x,t) \geq 0$ in the Clebsch-ansatz (3.21), which justifies the definition of the complex vortex field (3.19).

The *dislocation density tensor associated with the class* $\{\vec{l}, \vec{b}, \vec{m}\}$ [10] is the dyad

(3.22)
$$\boldsymbol{\alpha}_{\{l,b,m\}} = n_{\{...\}}(x,t)\,\vec{l} \otimes \vec{b}.$$

We get the *traditional, total dislocation density tensor* by superposing all classes:

(3.23)
$$\boldsymbol{\alpha} = \sum_{\{l,b,m\}} n_{\{...\}}(x,t)\,\vec{l} \otimes \vec{b}.$$

From (3.21) and (3.4) we obtain the *drift velocity of the dislocations of class* $\{\vec{l}, \vec{b}, \vec{m}\}$:

(3.24)
$$\vec{v}_{(d)\{...\}}(x,t) = \vec{v}_{\{...\}}(x,t) - \vec{v}_{(f)}(x,t).$$

It describes the motion of the dislocations with respect to the crystal lattice, i.e. it is associated with plastic deformation.

Having introduced the dislocation classes and its related fields (3.18) and (3.19), we result in a more refined description of dislocation dynamics than in traditional dislocation theory!

Obviously the dislocation classes are handled in an analogous way as before has been done with the carrier of the Cosserat fluid (see the fields Ψ, Ω and $\psi_{\{...\}}$, $\omega_{\{...\}}$, respectively). So, in our model the dynamics of the dislocated crystal can alternatively be looked upon as a sort of *multi-fluid model*. The vectors $\{\vec{l}, \vec{b}, \vec{m}\}$ are the Cosserat directors of that Cosserat fluid which is associated with the dislocation class $\{\vec{l}, \vec{b}, \vec{m}\}$.

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[10] Partial torsion due to class $\{\vec{l}, \vec{b}, \vec{m}\}$.

3.3. Thermodynamics of plasticity within LF

Looking at thermal effects of plasticity, the Cosserat fluid will further be endowed with the complex *thermion field* as the most fundamental variable of TIP within LF [5–10]:

$$(3.25) \qquad \chi(x,t) = \sqrt{T(x,t)}\exp(i\eta(x,t)).$$

It gives rise to the definition of the *absolute temperature*

$$(3.26) \qquad T(x,t) = \chi^*(x,t)\,\chi(x,t) \geq 0.$$

The phase function $\eta(x,t)$ is associated with the deviation of the irreversible heat transport process from local equilibrium [5, 6, 7]. Dissipation of mechanical energy during plastic deformation will be modelled as an *irreversible energy transfer* from mechanical to thermal degrees of freedom, i.e. from the matter field Ψ (Eq. (3.1)) of the Cosserat fluid and the dislocation fields $\psi_{\{lbm\}}$ (Eq. (3.18)) on the one hand to the thermion field χ (Eq. (3.25)) on the other hand. This transfer can be modelled in different ways: A direct coupling between the dislocation fields and the thermion field is discussed by Azirhi [22]. Another approach takes account of supplementary variables, which we call *transfer variables* [21].

4. The construction of the Lagrangian

4.1. The ideal hydroelastic fluid

Being a constitutive element of our Cosserat fluid, we start from the *Lagrangian of an ideal hydroelastic fluid* [24]:

$$(4.1) \qquad l_{\text{fluid}} = -\varrho\left[(\partial_t\Phi + \Lambda\partial_t M) + \frac{1}{2}(\nabla\Phi + \Lambda\nabla M)^2 + W(\varrho)\right]$$
$$= l_{\text{fluid}}(\varrho, \partial\Phi, \Lambda, \partial M),$$

where $W(\varrho)$ is the specific hydroelastic energy. This Lagrangian can equally well be expressed in terms of the complex matter field Ψ. The difference between both representations becomes essential only with regard to quantization, but not with respect to the present classical field theory. The form (4.1) is the simpler one for our purpose.

The ELEqs. associated with the variation of the variables ϱ, Φ, Λ, M are:

$$(4.2) \qquad \delta\Phi: \qquad \partial_t\varrho + \nabla\cdot[\varrho(\nabla\Phi + \Lambda\nabla M)] = 0,$$

$$(4.3) \qquad \delta\varrho: \qquad (\partial_t\Phi + \Lambda\partial_t M) + \frac{1}{2}(\nabla\Phi + \Lambda\nabla M)^2 - \left(\varrho\frac{\partial W}{\partial\varrho} + W\right) = 0,$$

$$(4.4) \qquad \delta\Lambda: \qquad [\partial_t + (\nabla\Phi + \Lambda\nabla M)\cdot\nabla]\Lambda = 0,$$

$$(4.5) \qquad \delta M: \qquad [\partial_t + (\nabla\Phi + \Lambda\nabla M)\cdot\nabla]M = 0.$$

Obviously (4.2) is the *mass balance equation* with the *mass flux density*

$$(4.6) \qquad \vec{J}_{(\varrho)} = \varrho(\nabla\Phi + \Lambda\nabla M)$$

and the *flow velocity*

$$(4.7) \qquad \vec{v}_{(f)} = \frac{\vec{J}_{(\varrho)}}{\varrho} = \nabla\Phi + \Lambda\nabla M.$$

Equation (4.3) is *Bernoulli's law* and (4.4), (4.5) together are equivalent with *Helmholtz's vortex law*. With regard to (4.7) the differential operator [...] in (4.4), (4.5) defines the substantial derivative. One can further easily show, that via Noether's theorem the Lagrangian (4.1) results in the correct balances for energy and momentum. Furthermore the mass balance (4.2) coincides with Noether's balance associated with the gauge group $\Psi \to \Psi e^{i\varepsilon}$, which is an invariance group of the Lagrangian ([11]).

4.2. The elastic crystal

We proceed to the Lagrangian of *a compatibly deforming, elastic crystal* without dislocations. Referring to our model of the compatible Cosserat fluid we are dealing with the deformation mode (I) of Subsec. 3.1. The *compatibility conditions for the holonomic and holonomically deforming Cosserat triads* are in compact and component form, respectively([12]):

$$(4.8) \qquad (\vec{a}_\kappa \cdot \nabla\vec{a}_\lambda)_{[\kappa,\lambda]} = 0, \qquad \left(A_\kappa^m \partial_m A_\lambda^j\right)_{[\kappa,\lambda]} = 0,$$

$$(4.9) \qquad \partial_t\vec{a}_\kappa + \vec{v}_{(f)} \cdot \nabla\vec{a}_\kappa - \vec{a}_\kappa \cdot \nabla\vec{v}_{(f)} = 0, \qquad \partial_t A_\kappa^k + v_{(f)}^m \partial_m A_\kappa^k - A_\kappa^m \partial_m v_{(f)}^k = 0.$$

The volume

$$(4.10) \qquad (\vec{a}_1, \vec{a}_2, \vec{a}_3) = \mathrm{Det}\,(A_\kappa^i) = A$$

spanned by the three directors is coupled with the mass density of the material carrier:

$$(4.11) \qquad A(x,t)\varrho(x,t) = m_0,$$

m_0 being the mass contained in the elementary cell of the crystal (atomic volume A).

([11]) One should keep in mind, that the Lagrangian (4.1) is exact. See footnote 1.
([12]) Latin and Greek indices refer to the external coordinate system x^k and to the internal director basis $\vec{a}_\kappa$, respectively.

By slightly modifying the ansatz (4.1) [13] and taking account of the kinematical constraints (4.8), (4.9), (4.11) by means of Lagrange multipliers $\vec{L}^{\kappa\lambda}$, $\vec{M}^\kappa$, N, we result in the *Lagrangian of the compatibly deforming, dislocation-free crystal*:

$$
\begin{aligned}
(4.12) \qquad l_{\text{elastic}} = & - \varrho\left[(\partial_t\Phi + \Lambda\partial_t M) + \frac{1}{2}\vec{v}_{(f)}^2 + W(\vec{a}_\kappa)\right] \\
& - \vec{L}^{\kappa\lambda}\cdot(\vec{a}_\kappa\cdot\nabla\vec{a}_\lambda)_{[\kappa,\lambda]} \\
& - \vec{M}^\kappa\cdot\left(\partial_t\vec{a}_\kappa + \vec{v}_{(f)}\cdot\nabla\vec{a}_\kappa - \vec{a}_\kappa\cdot\nabla\vec{v}_{(f)}\right) \\
& - N(\Lambda\varrho - m_0) \\
& - \vec{K}\cdot\left(\vec{v}_{(f)} - (\nabla\Phi + \Lambda\nabla M)\right) \\
= & \; l_{\text{elastic}}(\varrho, \partial\Phi, \Lambda, \partial M, \vec{v}_{(f)}, \vec{L}^{\kappa\lambda}, \vec{M}^\kappa, N, \vec{K}).
\end{aligned}
$$

It is formulated within the *model of the compatible Cosserat fluid* and is absolutely exact [14]. The variable $\vec{v}_{(f)}$ in the first and third row on the right-hand side of the equation has to be read as the Clebsch-ansatz (4.7). However, this results in a Lagrangian of the second order [15]. So, in order to keep the formalism within the first order, we prefer to insert the Clebsch-ansatz by means of another Lagrange multiplier $\vec{K}$ (last row) and to join $\vec{v}_{(f)}$ to the set of independent variational variables. One can show by means of the set of Euler–Lagrange equations and by means of Noether's energy and momentum balances, that (4.12) really describes the dynamics of the dislocation-free, elastically deforming crystal. It is a remarkable fact, that we again result in the mass balance (4.2) and that the velocity field of the deformation process is defined from this balance *without making use of a displacement field* (Eq. (4.7)). From this point of view we are well prepared to proceed to the plastically deformed crystal, i.e. to the incompatible Cosserat fluid.

4.3. The dislocated crystal

In order to take account of dislocations in our Cosserat fluid model we have to liberate the system from the kinematical constraints (4.8), (4.9):

$$
(4.13) \qquad \alpha = (\vec{a}_\kappa\cdot\nabla\vec{a}_\lambda)_{[\kappa,\lambda]} \neq 0, \qquad \alpha_{\kappa\lambda}{}^j - \left(A_\kappa^m\partial_m A_\lambda^j\right)_{[\kappa,\lambda]} = 0,
$$

$$
\begin{aligned}
(4.14) \qquad & \mathbf{J}_{(d)} = -\left(\partial_t\vec{a}_\kappa + \vec{v}_{(f)}\cdot\nabla\vec{a}_\kappa - \vec{a}_\kappa\cdot\nabla\vec{v}_{(f)}\right) \neq 0, \\
& J_{(d)\kappa}{}^k + \left(\partial_t A_\kappa^k + v_{(f)}^m\partial_m A_\kappa^k - A_\kappa^m\partial_m v_{(f)}^k\right) = 0.
\end{aligned}
$$

---

[13] $W(\varrho) \Rightarrow W(\vec{a}_\kappa, \kappa = 1, 2, 3)$.

[14] The most common form "density of kinetic energy minus density of the elastic energy" is but an approximate Lagrangian of the elastically deforming body (see footnote 1).

[15] Last term in the third row.

Formally α and $\mathbf{J}_{(d)}$ are the *incompatibility tensors* of the system. Physically these quantities have to be identified as follows: α is the *total dislocation density tensor*, which has to be understood as the *superposition* (3.23) *of dislocations of the different dislocation classes*:

$$(4.15) \qquad \alpha = \sum_{\{l,b,m\}} n_{\{\dots\}}(x,t)\, \vec{l} \otimes \vec{b}, \qquad \alpha^{\mu j} = \sum_{\{l,b,m\}} n_{\{\dots\}}(x,t)\, l^{\mu} b^{j}.$$

The tensor α can be taken as a third rank or a second rank tensor[16].

$$(4.16) \qquad \alpha^{\mu j} = \varepsilon^{\mu \kappa \lambda} \alpha_{\kappa \lambda}{}^{j}, \qquad \alpha_{\kappa \lambda}{}^{j} = \frac{1}{2} \varepsilon_{\mu \kappa \lambda} \alpha^{\mu j}.$$

$\mathbf{J}_{(d)}$ is the density tensor of the *drift dislocation flux*, which together with the *convective flux* $\mathbf{J}_{(f)}$ results in the total dislocation flux $\mathbf{J}$,

$$(4.17) \qquad \mathbf{J} = \mathbf{J}_{(f)} + \mathbf{J}_{(d)},$$

$$(4.18) \qquad \mathbf{J}_{(f)} = -\vec{v}_{(f)} \times \alpha, \qquad J_{(f)\kappa}{}^{j} = -\varepsilon_{\kappa \mu \nu} v_{(f)}^{\mu} \alpha^{\nu j}.$$

The drift flux is a *superposition of the partial drift fluxes associated with the dislocation classes*:

$$(4.19) \qquad
\begin{aligned}
\mathbf{J}_{(d)} &= - \sum_{\{l,b,m\}} \vec{v}_{(d)\{l,b,m\}} \times \alpha_{\{l,b,m\}}, \\
J_{(d)\kappa}{}^{j} &= - \sum_{\{l,b,m\}} \varepsilon_{\kappa \mu \nu} v_{(d)\{l,b,m\}}^{\mu} \alpha_{\{l,b,m\}}{}^{\nu j}.
\end{aligned}$$

Here $\vec{v}_{(f)}$ and $\vec{v}_{(d)\{l,b,m\}}$ are the *flux velocity of the material carrier* and the *drift velocities of the dislocations of classes* $\{\vec{l}, \vec{b}, \vec{m}\}$ respectively, defined from the matter and dislocation fields by Eqs. (3.4), (3.24), (3.21).

By means of the kinematical constraints (4.13), (4.14) and using the expressions (4.15), (4.17), (4.18), (4.19) and substituting the definitions (3.4), (3.24), (3.21) for the velocities, we finally result in *kinematical constraints for the dynamical eigenstress problem of a crystal with dislocations as well as for the plastically deforming crystal*. In the case of the dynamical eigenstress problem the dislocation fields $\psi_{\{\dots\}}$ are different from zero but the dislocation drift velocities $\vec{v}_{(d)\{\dots\}}$ vanish (sessile dislocations). The Cosserat triads are anholonomic. Furthermore in the case of plastic deformation the Cosserat triads are deforming anholonomically, i.e. they are only partially dragged along with the carrier's flow.

---

[16] A more refined consideration may distinguish between tensors and tensor densities according to the permutation symbols $\epsilon^{\mu \kappa \lambda}$ and $\epsilon_{\mu \kappa \lambda}$ which – precisely speaking – are no tensors but "tensor densities of weight 1 and -1", respectively [25].

The dislocations are moving with respect to the crystal, i.e. their drift velocities $v_{(d)\{l,b,m\}}$ are different from zero.

We are now prepared to write down the *pure mechanical Lagrangian of the dynamical eigenstress problem* of a crystal with sessile dislocations, and – simultaneously – of a *plastically deforming crystal* with moving dislocations. The Lagrangian (4.12) of the compatible Cosserat fluid will slightly be extended:

$$(4.20) \qquad l_{\text{plastic}} = -\varrho \left[(\partial_t \Phi + \Lambda \partial_t M) + \frac{1}{2} \vec{v}_{(f)}^2 \right]$$

$$- \varrho \left[\frac{1}{2} \Theta^{\kappa\lambda} D_t \vec{a}_\kappa \cdot D_t \vec{a}_\lambda + W(\vec{a}_\kappa, \nabla \vec{a}_\kappa) \right]$$

$$- \sum_{\{l,b,m\}} m_{\{l,b,m\}} n_{\{l,b,m\}} \left[(\partial_t \varphi_{\{l,b,m\}} + \lambda_{\{l,b,m\}} \partial_t \mu_{\{l,b,m\}}) + \frac{1}{2} \vec{v}_{\{l,b,m\}}^2 + \varepsilon_{\{l,b,m\}} \right]$$

$$+ L^{\kappa\lambda}{}_j \left[\frac{1}{2} \epsilon_{\kappa\lambda\mu} \sum_{\{l,b,m\}} (n_{\{l,b,m\}} l^\mu b^j) - (A^m_\kappa \partial_m A^j_\lambda)_{[\kappa,\lambda]} \right]$$

$$+ M^\kappa{}_j \left[\epsilon_{\kappa\lambda\mu} \sum_{\{l,b,m\}} ((v^\lambda_{\{l,b,m\}} - v^\lambda_{(f)}) n_{\{l,b,m\}} l^\mu b^j) - \left(\partial_t A^j_\kappa + v^m_{(f)} \partial_m A^j_\kappa - A^m_\kappa \partial_m v^j_{(f)} \right) \right]$$

$$- N \left[A\varrho - m_0 \right]$$

$$- \vec{K}_1 \cdot \left[\vec{v}_{(f)} - (\nabla\Phi + \Lambda\nabla M) \right]$$

$$- \sum_{\{l,b,m\}} \vec{K}_{2\{l,b,m\}} \cdot \left[\vec{v}_{\{l,b,m\}} - (\nabla\varphi_{\{l,b,m\}} + \lambda_{\{l,b,m\}} \nabla\mu_{\{l,b,m\}}) \right]$$

$$= l_{\text{plastic}}(\varrho, \partial\Phi, \Lambda, \partial M, \vec{a}_\kappa, \partial\vec{a}_\kappa, n_{\{l,b,m\}}, , \partial\varphi_{\{l,b,m\}}, \lambda_{\{l,b,m\}}, \partial\mu_{\{l,b,m\}},$$
$$\vec{v}_{(f)}, \partial\vec{v}_{(f)}, \vec{v}_{\{l,b,m\}}, \partial\vec{v}_{\{l,b,m\}}, L^{\kappa\lambda}{}_j, M^\kappa{}_j, N, \vec{K}_1, \vec{K}_{2\{l,b,m\}}).$$

The different terms are written in the compact tensor form and in the index form, respectively, depending on the most lucid form of the respective terms. The arguments which will take part in the variational procedure, are listed explicitly in $l_{\text{plast}}(...)$ in the last row. The plus signs in front of the multipliers L and M are chosen in succession to the respective terms in Eq. (4.12). One should keep in mind, that the line vectors $\vec{l}$ and the Burgers vectors $\vec{b}$ of the dislocations (4-th and 5-th row) are involved in the variation of the Cosserat triads according to (3.16) and (3.7). In the 2-nd row there is involved the substantial derivative

$$(4.21) \qquad\qquad D_t = \partial_t + \vec{v}_{(f)} \cdot \nabla,$$

which is necessary according to the Galilean invariance of the Lagrangian.

The theory of elasto-plastic deformation based on the *Lagrangian* (4.20) *is a reversible, pure mechanical theory.* Especially the reversibility is due to the

time reversal invariance of l_{plast} (replace: $t \Rightarrow -t$, complex fields $\Rightarrow$ conjugated complex fields, i.e. phase functions $\Rightarrow$ opposite phase functions, velocities $\Rightarrow$ opposite velocities, multipliers $M, K_1, K_2 \Rightarrow$ opposite multipliers).

The rows in l_{plastic} are in turn associated with the dynamics of the different parts of our model.

1-ST ROW: *The dynamics of the material carrier:*

As compared with (4.12) the elastic potential is now joint with the Cosserat triads. The second term defines the translational kinetic energy. The ansatz describes in the continuum picture the dynamics of a flow of free particles.

2-ND ROW: *The dynamics of the Cosserat directors:*

The first term defines the kinetic energy of the Cosserat triads. It is associated with the micro-inertia of the triads (tensor Θ). W is the elastic potential associated with the elastic energy of the crystal. As compared with l_{elast} (see (4.12)) this potential is supplemented by the lattice curvature – involved in $\nabla \vec{a}_\kappa$ – in order to account for moment stresses, which are a natural ingredient of the theory of Cosserat continua and of the dislocation theory. The 2-nd row describes the elastodynamics of the crystal.

3-RD ROW: *The dislocation dynamics of the different classes:*

For the dislocation dynamics we assume again the continuum model of a flowing medium. As already mentioned at the end of in Subsec. 3.2 we are thus formally dealing with a "multi-fluid" system. The quantity $m_{\{l,b,m\}}$ is the effective mass of the dislocations. It is related with the inertia of dislocations. The quadratic term is the kinetic energy of the dislocations, whereas $\varepsilon_{\{l,b,m\}}$ is the self-energy of the dislocation kernel [12]. The latter one will become important in a later stage of the theory, when creation and annihilation of dislocations will be taken into account.

Using the Lagrange multipliers the next rows take account of the *kinematical couplings* discussed above:

4-TH ROW: The kinematical coupling of the dislocations of all classes with the torsion involved in the field of Cosserat triads.

5-TH ROW: The kinematical coupling between the Cosserat triads and the carrier's flow via the motion of the dislocation of all classes.

6-TH ROW: The kinematical coupling of the triads with the mass of the carrier.

These three terms given rise to a dynamical coupling between the material flow (material carrier) of the medium, its elasticity (Cosserat triads) and its dislocations.

Finally a few more *formal constraints* are involved:

7-TH ROW: A formal variational constraint between the carrier's flow velocity and its Clebsch potentials.

Using this constraint we preserve again a first order Hamilton's principle (see the last term in the 5-th row).

8-TH ROW: A formal variational constraint between the dislocation flow velocities and its Clebsch potentials.

This constraint could be avoided. It is introduced because of a formal symmetry between the velocities of all "partial fluids".

The Lagrangian (4.20) completely describes the unrestricted dynamics of *freely moving dislocations* due to elastic stresses; the *Cosserat triads are the transmitters of the elastic stresses*. Under external load the dislocation motion gives rise to an accelerating flow of the material carrier, i.e. to an accelerating plastic flow of the crystal. For a more detailed discussion we refer to the forthcoming papers [22].

In reality there is a pinning of dislocations due to the discrete crystal lattice (Peierls potential) and due to the pinning of dislocations at a lot of different obstacles disturbing the perfectness of the crystal. So, in order to cause sessile dislocations to move, the local driving forces acting on dislocations (Peach–Koehler force) have to overcome particular thresholds. By means of the following considerations we are able to involve these effects into our Lagrangian field theory of plastic deformation ([17]):

The density of the Peach–Koehler force on dislocations of the class $\{\vec{l}, \vec{b}, \vec{m}\}$ is given by

$$(4.22) \qquad \vec{\Gamma}_{\{l,b,m\}} = n_{\{l,b,m\}}\, \vec{l} \times (\boldsymbol{\sigma} \cdot \vec{b});$$

$\boldsymbol{\sigma}$ is the local elastic stress tensor (1.3). Projecting $\vec{\Gamma}_{\{l,b,m\}}$ onto the glide plain (normal $\vec{m}$) we result in the relevant driving force acting on these dislocations:

$$(4.23) \qquad \vec{\tau}_{\{l,b,m\}} = \vec{m} \times \vec{\Gamma}_{\{l,b,m\}} \times \vec{m} = (1 - \vec{m} \otimes \vec{m}) \cdot \vec{\Gamma}_{\{l,b,m\}}\,.$$

By definition of the P.K. force the vector $\vec{\tau}_{\{l,b,m\}}$ is perpendicular to the dislocation line. This stress gives rise to dislocation motion if and only if it overcomes the critical stress $\tau^c_{\{l,b,m\}} > 0$, which is assumed to be characteristic for each class and for each type of stability barrier:

$$(4.24) \qquad |\vec{\tau}_{\{l,b,m\}}| < \tau^c_{\{l,bm\}} \Leftrightarrow \vec{v}_{(d)\{l,b,m\}} = 0 \Leftrightarrow \text{sessile dislocations,}$$

$$(4.25) \qquad |\vec{\tau}_{\{l,b,m\}}| \geq \tau^c_{\{l,b,m\}} \Leftrightarrow \vec{v}_{(d)\{l,b,m\}} \neq 0 \Leftrightarrow \text{moving dislocations.}$$

Both cases can be joint together in one equation by means of Heaviside's function ([18]):

$$(4.26) \qquad (\vec{v}_{(d)\{l,b,m\}} \cdot \vec{v}_{(d)\{l,b,m\}}) H(\tau^c_{\{l,b,m\}}{}^2 - \vec{\tau}_{\{l,b,m,\}} \cdot \vec{\tau}_{\{l,b,m\}}) = 0\,.$$

Obviously this equation is solved by the inequalities (4.24), (4.25).

([17]) In a more general context these questions are related with dynamical stability of the dislocation dynamics. See the remarks in Subsec. 2.5.

([18]) $H(z) = 0$ or 1 for $z \leq 0$ or $z > 0$.

Taking Eq. (4.26) into account by means of another Lagrange multiplier we pass from (4.20) to a *Lagrangian which* – in a first and lump-sum way – *takes account of a critical stress* in the phenomenological stress-strain curve of an elasto-plastic material. Locally a free motion of dislocations takes place whenever and wherever the inequality (4.25) holds. Otherwise the motion of the dislocations stops abruptly; the dislocations are pinned. Phenomenologically there are spatial regions in the deforming material where we get plastic or pure elastic deformations according to the ineqalities (4.25) or (4.24), respectively. Moving dislocations give rise to a reduction of elastic strains till we arrive at the situation (4.24), where the plastic flow stops. However, we are still dealing with a reversible, purely mechanical theory. The thresholds $\tau^c_{\{l,b,m\}}$ are not yet related with dissipation!

5. Perspectives

The theory of elasto-plastic deformation and of dislocation dynamics presented in this paper will be extented towards several goals:

The creation of dislocations *via* the Frank–Read sources can be involved in various ways: With regard to the activation barrier of Frank–Read sources there is an analogy with the relations (4.24-26). Another possibility is due to analogies between a dislocated crystal and a spin system [22, 23].

Dislocation reactions between dislocations of different classes are analogous with chemical reactions. The dynamics of the latter ones is already involved into LF [7]. Furthermore the transition from immobile to mobile dislocations and vice versa can be looked upon as creation and annihilation processes [22].

The Lagrangian (4.20) will be extended towards dissipative dislocation dynamics. A first approach is based on a direct coupling between the dislocation fields and the thermion field: Friction gives rise to a transition of the dislocations from the mobile to the immobile state [22]. Alternatively we shall attack the difficult problem of dislocation motion with friction by means of *transfer variables*, which manage the energy transfer from the mechanical to the thermal degrees of freedom. Using this method we already succeeded in the dissipation problem in point mechanics [21]. A third approach tries to take advantage of the methods of the gauge theory [20].

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