Mesoscopic theory of microcracks

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THE MESOSCOPIC CONCEPT is a way to deal with complex materials with an internal structure within continuum mechanics. It consists of extending the domain of the balance equations by mesoscopic variables and of introducing a local distribution function of these variables as a statistical element. In our case microcracks are modelled as penny-shaped and are completely characterized by their diameter and the unit normal to the crack surface. Two examples of crack dynamics are given as well as a possible definition of a damage parameter. Orientational order parameters (fabric-alignment tensors) are defined and balance-like dynamic equations for them are derived.

1. A model of microcracks

MACROSCOPIC FAILURE OF BRITTLE materials is initiated by the propagation of microcracks. In a simple model the microcrack is described as a flat, rotationally symmetric surface, a so-called penny-shaped crack. In addition we make here the following simplifying assumptions:

1. The diameter of the cracks is much smaller than the linear dimensions of the continuum element. Under this assumption the cracks can be treated as an internal structure of the continuum element. The cracks are assumed to be small enough so that there is a whole distribution of crack sizes and orientations in the volume element.

2. The cracks are fixed to the material. Therefore their motion is coupled to the motion of representative volume elements.

3. The cracks cannot rotate independently of the material, i.e. if they have a nonzero rotation velocity at all, this rotation velocity is determined by the antisymmetric part of the time derivative of the deformation gradient of the surrounding material and it does *not* depend on crack length and orientation. All cracks within a volume element move and rotate with the same velocity.

4. The number of cracks is fixed, there is no production of cracks, but very short cracks are preexisting in the virgin material.

5. The cracks cannot decrease their area, but can only enlarge, meaning that cracks cannot heal.

To summarize our model, the microcrack is characterized by a unit vector **n** representing the orientation of the surface normal and by the radius l of the circular crack surface. These parameters will be taken as the additional variables in the mesoscopic theory.

2. Different approaches to damage mechanics and the mesoscopic concept

There are two principally different possibilities to deal with complex materials within continuum mechanics: the first way is to introduce additional fields depending on position and time. These fields can be any kind of internal variables [1, 2], or damage parameters [3, 4], and damage tensors (fabric tensors) [5, 6]. In damage mechanics such additional macroscopic variables have been introduced in many different cases of materials with internal structure like liquid crystals [7, 8], polymer solutions [9, 10] and others. The other way is a so-called mesoscopic theory. The idea is to enlarge the domain of the field quantities by an additional variable, characterizing the internal degree of freedom connected with the internal structure of the material. Field quantities are introduced, which are defined on an enlarged space $\mathbb{R}^3_x \times \mathbb{R}_t \times M$. The manifold M is given by the set of values the internal degrees of freedom can take. In our case the internal degrees of freedom are the different sizes l and orientations **n** of microcracks. We call this way of dealing with the internal structure of complex materials a mesoscopic theory, because it includes more information than a macroscopic theory on $\mathbb{R}^3_x \times \mathbb{R}_t$, but less than a microscopic one on the molecular level. The domain of the mesoscopic field quantities $\mathbb{R}^3_x \times \mathbb{R}_t \times M$ is called the mesoscopic space.

Macroscopic quantities are calculated from mesoscopic ones as averages over crack sizes and crack orientations. The spatial distribution of cracks is not relevant in the sense that the resulting macroscopic quantities are still field quantities depending on position and time. For a treatment of the spatial distribution of cracks and a possible coarsening process see [11].

In contrast to spatial averaging introduced in [12], a nonlocal generalization of the classical Weibull theory, the averages in mesoscopic theory are local in space. They are averages over different microcrack sizes and orientations in a volume element.

Scaling properties [13] are completely out of scope of the whole mesoscopic theory. They result from microscopic statistical considerations. Statistical theories of fracture describe the breakdown of material as a second order phase transition [14, 13], as well as a first order phase transition [15–17].

We will apply now the mesoscopic concept to a damaged material with microcracks. The crack length can take values between a minimal length l_m of the smallest preexisting cracks and a maximal length l_M, which is limited by the linear dimension of the continuum element. The orientation of the unit vector $\mathbf{n}$ can be given by an element of the unit sphere S^2. Therefore in the example of microcracks the manifold M is given by $[l_m, l_M] \times S^2$. The change velocities of the mesoscopic variables l and $\mathbf{u} := \dot{\mathbf{n}}$ are defined in such a way that for $\Delta t \to 0$ we have

$$(2.1) \qquad l(t + \Delta t) = l(t) + \dot{l}\Delta t \,, \qquad \mathbf{n}(t + \Delta t) = \mathbf{n}(t) + \mathbf{u}\Delta t$$

at later times $t + \Delta t$. The rotation velocity $\mathbf{u}$ and the length change velocity $\dot{l}$ are the components in spherical coordinates of the crack velocity $\mathbf{v}_l$ introduced in [18]. In this previous paper [18] the set of additional mesoscopic variables $\mathbf{n}$ and l was called directional variable.

Beyond the use of additional variables, the mesoscopic concept introduces a statistical element, the so-called mesoscopic distribution function. In our case this is a distribution of crack lengths and orientations in the continuum element at position $\mathbf{x}$ and time t, called here crack distribution function (CDF). The distribution function is the probability density of finding a crack of length l and orientation $\mathbf{n}$ in the continuum element.

3. Mesoscopic balance equations

Now such fields as mass density, momentum density, angular momentum density, and energy density are defined on the mesoscopic space. For distinguishing these fields from the macroscopic ones we add the word "mesoscopic". In addition we introduce the crack number density N as an extensive quantity. The mesoscopic crack number density $N(l, \mathbf{n}, \mathbf{x}, t)$ is the number density, counting only cracks of length l and orientation $\mathbf{n}$. For this crack number density there is a balance equation too, as it is an extensive quantity. The crack number density can be prescribed independently of the mass density, although the motion of cracks is coupled to the motion of surrounding material in our model. Therefore

we distinguish here between the two fields: mass density ρ and number density N, although they have the same equation of motion and were not distinguished in an earlier paper [18].

3.1. Definition of the distribution function

Due to its definition as probability density, the distribution function is the number fraction

(3.1)
$$f(l, \mathbf{n}, \mathbf{x}, t) = \frac{N(l, \mathbf{n}, \mathbf{x}, t)}{N(\mathbf{x}, t)},$$

in volume elements, where the number density $N(\mathbf{x}, t)$ is non-zero. Here $N(\mathbf{x}, t)$ is the macroscopic number density of cracks of any length and orientation. Since the distribution function in Eq. (3.1) is not well defined if $N(\mathbf{x}, t) = 0$, we define in addition that in this case $f(l, \mathbf{n}, \mathbf{x}, t) = 0$. Since there is no creation of cracks in our model, the distribution function will be zero for all times in these volume elements. In all other volume elements with a nonzero crack number it is normalized

(3.2)
$$\int_{l_m}^{l_M} \int_{S^2} f(l, \mathbf{n}, \mathbf{x}, t) l^2 d^2 n dl = 1.$$

3.2. Balance equations of mass, momentum, angular momentum, and energy

For the mesoscopic densities the local balance equations have been derived from the macroscopic global ones [18–21]. The macroscopic balance equations express the fact that the extensive macroscopic quantities within a region G can change due to a flux over the boundary ∂G and due to production and supply within G. This results in the general form of a global balance equation

(3.3)
$$\frac{d}{dt} \int_G \mathbf{X} d^3 x d n l^2 dl = \int_{\partial G} \varphi_{\mathbf{X}}(\cdot) da + \int_G \Sigma_X(\cdot) d^3 x d n l^2 dl.$$

A generalized Reynolds transport theorem on the mesoscopic space, analogous to the one in [22], is used to transform the time derivative, and a generalized Gauss theorem is applied. The boundary ∂G of G consists of parts in the position space, in the orientation space, and in the length interval. In regular points of the continuum we get the general form of a local mesoscopic balance equation [18] with the abbreviation $(\cdot) = (l, \mathbf{n}, \mathbf{x}, t)$:

$$\frac{\partial}{\partial t}\mathbf{X}(\cdot) + \nabla_x \cdot [\mathbf{v}(\cdot)\mathbf{X}(\cdot) - \mathbf{S}(\cdot)] + \nabla_n \cdot [\mathbf{u}(\cdot)\mathbf{X}(\cdot) - \mathbf{R}(\cdot)]$$

$$+ \frac{1}{l^2}\frac{\partial}{\partial l}\left(l^2 i(\cdot)\mathbf{X}(\cdot) - \mathbf{R}_l(\cdot)\right) = \Sigma(\cdot),$$

where $\mathbf{R}$ and $\mathbf{R}_l$ are the non-convective fluxes over the orientational and length part of the boundary of G, and G is a region in $\mathbb{R}^3 \times S^2 \times [l_m, l_M]$. The derivative with respect to the mesoscopic variable $(l, \mathbf{n})$ is represented in spherical coordinates. In the derivation of the local balance equation it has been supposed that there is no flux over the boundary of the total mesoscopic space:

(3.4)
$$\int\limits_{-\infty}^{\infty} \int\limits_{S^2} \int\limits_{l_m}^{l^M} \nabla \cdot \varphi_{\mathbf{X}}(\cdot) d^3x \, d\mathbf{n} \, l^2 dl = 0.$$

Otherwise such a non-zero flux term (3.4) could be interpreted as an additional source term on the right-hand side of the equation.

Explicitly we have:

Balance of mass

(3.5)
$$\frac{\partial}{\partial t}\varrho(\cdot) + \nabla_x \cdot \{\varrho(\cdot)\mathbf{v}(\mathbf{x}, t)\} + \nabla_n \cdot \{\varrho(\cdot)\mathbf{u}(\mathbf{x}, t)\} + \frac{1}{l^2}\frac{\partial}{\partial l}\left(l^2 i\varrho(\cdot)\right) = 0.$$

Balance of momentum

(3.6)
$$\frac{\partial}{\partial t}[\varrho(\cdot)\mathbf{v}(\mathbf{x}, t)] + \nabla_x \cdot \left[\mathbf{v}(\mathbf{x}, t)\varrho(\cdot)\mathbf{v}(\mathbf{x}, t) - \mathbf{t}^\top(\cdot)\right]$$

$$+ \nabla_n \cdot \left[\mathbf{u}(\mathbf{x}, t)\varrho(\cdot)\mathbf{v}(\mathbf{x}, t) - \mathbf{T}^\top(\cdot)\right] + \frac{1}{l^2}\frac{\partial}{\partial l}\left(l^2 i\varrho(\cdot)\mathbf{v}(\mathbf{x}, t) - \boldsymbol{\tau}(\cdot)\right)$$

$$= \varrho(\cdot)\mathbf{f}(\cdot).$$

Here $\mathbf{f}(\cdot)$ is the external acceleration density, $\mathbf{t}^\top(\cdot)$ the transposed mesoscopic stress tensor, and $\mathbf{T}^\top(\cdot)$ the transposed stress tensor on orientation space (non-convective momentum flux in orientation space), $\boldsymbol{\tau}(\cdot)$ is the momentum flux vector with respect to the crack length variable. We introduced already the assumption that the material velocity $\mathbf{v}$ and the rotational velocity $\mathbf{u}$ are the same for cracks of all orientations and lengths.

Angular momentum

The balance of angular momentum has to be taken into account as an additional equation independent of the balance of momentum, because there is an

internal angular momentum due to crack rotations. The total angular momentum

$$(3.7) \qquad \mathbf{S}(\mathbf{x}, t) := \mathbf{x} \times \mathbf{v}(\mathbf{x}, t) + \mathbf{s}(\cdot)$$

is the sum of the moment of momentum and the internal angular momentum.

$$(3.8) \qquad \frac{\partial}{\partial t}[\varrho(\cdot)\mathbf{S}(\cdot)] + \nabla_x \cdot \left[\mathbf{v}(\mathbf{x}, t)\varrho(\cdot)\mathbf{S}(\cdot) - (\mathbf{x} \times \mathbf{T}(\cdot))^\top - \mathbf{\Pi}^\top(\cdot) \right]$$

$$+ \nabla_n \cdot \left[\mathbf{u}(\mathbf{x}, t)\varrho(\cdot)\mathbf{S}(\cdot) - (\mathbf{x} \times \boldsymbol{\tau}(\cdot))^\top - \boldsymbol{\pi}^\top(\cdot) \right]$$

$$+ \frac{1}{l^2}\frac{\partial}{\partial l}\left(l^2 l \varrho(\cdot)\mathbf{S}(\cdot) - \boldsymbol{\omega}(\cdot) \right) = \varrho(\cdot)\mathbf{x} \times \mathbf{k}(\cdot) + \varrho(\cdot)\mathbf{g}.$$

Here $\mathbf{n} \times \mathbf{g}$ is the vector of couple forces (acting on crack orientation), the tensor $\mathbf{\Pi}$ is the surface torque, and $\boldsymbol{\pi}$ is the analogue with respect to orientation, and ω is the analogue with respect to crack length. These constitutive quantities appear in the non-convective fluxes in the position space, orientation space, and in the length interval, respectively. This equation can be simplified with the assumptions that the material velocity and the rotation velocity depend only on position and time $\mathbf{v}(\mathbf{x}, t)$ and $\mathbf{u}(\mathbf{x}, t)$.

However, the spin is only relevant, if the model allows for crack rotations independently of the rotations of material elements, and this is not the case in our simplified example dynamics.

Similarly the balance of energy can be given, which is omitted here and can be found in [18]. In all balance equations, in addition to the flux with respect to the position variable, there appear additional flux terms with respect to the additional mesoscopic variables crack orientation and length.

Balance of crack number

In our model the cracks move together with the material element. Therefore their flux is the convective flux, having a part in position space, a part in orientation space, and a part in the length interval. There is no production and no supply of crack number. Therefore we have for the crack number density N:

$$(3.9) \qquad \frac{\partial}{\partial t}N(\cdot) + \nabla_x \cdot \{N(\cdot)\mathbf{v}(\mathbf{x}, t)\} + \nabla_n \cdot \{N(\cdot)\mathbf{u}(\mathbf{x}, t)\} + \frac{1}{l^2}\frac{\partial}{\partial l}\left(l^2 l N(\cdot) \right) = 0.$$

In a fixed volume element this crack number density is proportional to the mass density, and therefore these two fields were not distinguished in an earlier paper [18].

We obtain from the mesoscopic balance of crack number density (3.9) a balance of the CDF $f(l, \mathbf{n}, \mathbf{x}, t)$, by inserting its definition (3.1):

(3.10)
$$\frac{\partial}{\partial t} f(l, \mathbf{n}, \mathbf{x}, t) + \nabla_x \cdot (\mathbf{v}(\mathbf{x}, t) f(l, \mathbf{n}, \mathbf{x}, t))$$

$$+ \nabla_n \cdot (\mathbf{u}(\mathbf{x}, t) f(l, \mathbf{n}, \mathbf{x}, t)) + \frac{1}{l^2} \frac{\partial}{\partial l} \left(l^2 \dot{l} f(l, \mathbf{n}, \mathbf{x}, t) \right)$$

$$= \frac{-f(l, \mathbf{n}, \mathbf{x}, t)}{N(\mathbf{x}, t)} \left(\frac{\partial}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla_x \right) N(\mathbf{x}, t)$$

$$= \frac{-f(l, \mathbf{n}, \mathbf{x}, t)}{N(\mathbf{x}, t)} \frac{dN(\mathbf{x}, t)}{dt} = 0.$$

The right-hand side is equal to zero, as for the co-moving observer the total number of cracks in a volume element does not change in time, as in our model no cracks are created. In our model all cracks in a volume element move with the translational velocity of the volume element $\mathbf{v}(\mathbf{x}, t)$ and rotate with the velocity $\mathbf{u} = \nabla \times \mathbf{v}(\mathbf{x}, t)$. Therefore the first three terms on the left-hand side can be summarized as a co-moving time derivative of the distribution function (the time derivative of an observer moving with the material elements) with the abbreviation d^c/dt:

(3.11)
$$\frac{\partial}{\partial t} f(l, \mathbf{n}, \mathbf{x}, t) + \mathbf{v}(\mathbf{x}, t) \cdot \nabla_x f(l, \mathbf{n}, \mathbf{x}, t) + \mathbf{u}(\mathbf{x}, t) \cdot \nabla_n f(l, \mathbf{n}, \mathbf{x}, t)$$

$$= \frac{d^c f(l, \mathbf{n}, \mathbf{x}, t)}{dt}.$$

If we assume in addition an incompressible motion $\nabla_x \cdot \mathbf{v} = 0$, we end up with the equation of motion for the CDF:

(3.12)
$$\frac{d^c f(l, \mathbf{n}, \mathbf{x}, t)}{dt} + \frac{1}{l^2} \frac{\partial}{\partial l} \left(l^2 \dot{l} f(l, \mathbf{n}, \mathbf{x}, t) \right) = 0.$$

This is not yet a closed differential equation for the CDF as long as no expression for the length change velocity of the crack $\dot{l}$ is given. An example of such a closed equation will be discussed later.

Macroscopic quantities are obtained from mesoscopic ones as averages with the CDF as probability density:

(3.13)
$$A(\mathbf{x}, t) = \int\limits_{l_m}^{l_M} \int\limits_{S^2} A(l, \mathbf{n}, \mathbf{x}, t) f(l, \mathbf{n}, \mathbf{x}, t) d^2 n l^2 dl.$$

Entropy balance

Besides these mesoscopic balances, the entropy balance is necessary for introducing the second law of thermodynamics. Because the production of mesoscopic entropy is not necessarily positive for each crack length and orientation, the entropy balance is only interesting in its macroscopic form

$$(3.14) \qquad \frac{\partial}{\partial t}[\varrho(\mathbf{x},t)\eta(\mathbf{x},t)] + \nabla_x \cdot [\varrho(\mathbf{x},t)\eta(\mathbf{x},t)\mathbf{v}(\mathbf{x},t) + \boldsymbol{\phi}(\mathbf{x},t)] = \varrho(\mathbf{x},t)\sigma(\mathbf{x},t)$$

(η = specific entropy density, $\boldsymbol{\phi}$ = entropy flux density, σ = entropy production density). The second law is expressed by the *dissipation inequality*

$$(3.15) \qquad\qquad\qquad\qquad \sigma(\mathbf{x},t) \geq 0.$$

The set of balance equations is not a closed system of equations, constitutive equations for mesoscopic quantities are needed. The domain of the constitutive mappings is the state space; here a mesoscopic one. There are the possibilities that the mesoscopic state space includes *only* mesoscopic quantities, or that it includes mesoscopic *and* macroscopic quantities, and there are examples where such mixed state spaces cannot be avoided [23]. (For instance in the case of liquid crystals the macroscopic alignment tensor is included in a mesoscopic state space. This is necessary to account for the orienting mean field of surrounding ordered particles. Otherwise it is not possible to describe the phase transition from the isotropic phase to the ordered liquid crystalline phase) Constitutive equations have to be such that the second law of thermodynamics is fulfilled by any solution of the macroscopic balance equations with the constitutive equations inserted [24]. This requirement restricts the possible constitutive functions.

Finally, even for the exploitation of the dissipation inequality, which is possible only on the macroscopic level, the choice of variables can be motivated by the mesoscopic background [25, 26]. A relevance of these variables could not be guessed from a purely macroscopic theory.

4. Damage parameter and order parameters

4.1. Definition of a damage parameter

The damage parameter is introduced as a macroscopic quantity growing with progressive damage in such a way that it should be possible to relate the change of material properties to the growth of the damage parameter. We define the damage parameter as the fraction of cracks, which have reached a certain length L. The idea is that cracks of this and larger sizes considerably decrease the strength

of the material, and therefore their fraction is a measure of the damage. This idea is related to the slender bar model of KRAJCINOVIC [5] (especially useful in one-dimensional crack problems), where the damage parameter is introduced as the number of "broken bars" in the sample,

$$(4.1) \qquad D(\mathbf{x}, t) = \int\limits_{L} \int\limits_{S^2} f(l, \mathbf{n}, \mathbf{x}, t) d^2 n l^2 dl.$$

In this definition of the damage parameter the possibility of cracks of any length $(l_M \to \infty)$ is included. This is consistent with many possible laws of crack growth, where the crack does not stop growing.

More sophisticated definitions, taking into account the orientational distribution too, are possible and will be discussed elsewhere. Another measure of damage which could be introduced is the average crack length [27].

4.2. Length order parameters

From the mesoscopic distribution function two different kinds of moment series can be built because of the dependence on crack length and on crack orientation. We can introduce moments of the distribution function with respect to crack length:

$$(4.2) \qquad \int\limits_{l_m}^{l_M} f(l, \mathbf{n}, \mathbf{x}, t) P_k(l) l^2 dl =: p_k(\mathbf{n}, \mathbf{x}, t),$$

where $P_k(l)$ are polynomials being orthogonal with respect to the measure $l^2 dl$:

$$(4.3) \qquad \int\limits_{l_m}^{l_M} P_i(l) P_j(l) l^2 dl = \delta ij.$$

The moments introduced in Eq. (4.2) still depend on crack orientation. Averaging over all orientations gives macroscopic fields, the length order parameters:

$$(4.4) \qquad \pi_k(\mathbf{x}, t) = \int\limits_{S^2} P_k(\mathbf{n}, \mathbf{x}, t) d^2 n.$$

In the following we will investigate the moments of the distribution function with respect to crack orientation.

4.3. Orientational order parameters

We can introduce the following set of alignment-fabric tensors of successive tensorial order

$$(4.5) \qquad a^{(k)}(\mathbf{x}, t) := \int\limits_{l_m}^{l_M} \int\limits_{S^2} f(l, \mathbf{n}, \mathbf{x}, t) \, \underbrace{\overline{\mathbf{n} \circ \dots \circ \mathbf{n}}}_{k} \, l^2 dl d^2 n,$$

where $\overline{\cdots}$ denotes the symmetric irreducible part of a tensor [28]. Remarkable, that only the even order tensors appear in the series because the microcracks are represented by axial vectors, the unit normal to the crack surface, i.e. $\mathbf{n}$ and $-\mathbf{n}$ are not distinguished. Due to this symmetry all odd order moments vanish. The tensors defined above are macroscopic quantities. We want to call them alignment-fabric-tensors. Originally tensorial damage parameters were introduced on a purely statistical ground, without a mesoscopic foundation and were called "fabric tensors of the second kind" in damage mechanics (see KANATANI [6] or KRAJCINOVIC [5]). The alignment-fabric-tensors represent the orientational distribution of microcracks, but do not take into account their lengths. They have to be distinguished from the scalar damage parameter which is a measure of the growth of cracks. These alignment-fabric tensors form a whole set of internal variables in the sense of thermodynamics.

The alignment-fabric tensors are a measure of the deviation of the crack orientation distribution from isotropy. They are all zero, if all crack orientations are equally probable, and at least some alignment-fabric tensors are nonzero in case of anisotropic distributions. The orientation distribution of cracks and therefore the alignment-fabric tensors become important in the dynamics of the crack distribution. There are usually the specimen geometry and loading conditions rotation symmetric around an axis $\mathbf{d}$ (uniaxial conditions). It is reasonable to assume that also the distribution of crack orientations is rotationally symmetric around the same axis $\mathbf{d}$. Then, for symmetry reasons, all alignment-fabric tensors of different orders can be expressed in terms of scalar orientational order parameters $S^{(k)}$ and the unit vector $\mathbf{d}$ in the following way:

$$(4.6) \qquad a^{(k)} = S^{(k)} \underbrace{\overline{\mathbf{d} \circ \dots \circ \mathbf{d}}}_{k} \qquad (k = 2, 4, \dots),$$

where the order parameters $S^{(k)}$ are one in case of total alignment (the microcracks stand parallel) and zero for randomly oriented cracks.

4.4. Equations of motion for the alignment-fabric tensors and for the damage parameter

In general a coupled set of equations of motion for the alignment-fabric tensors of different order can be derived from the differential equation for the crack distribution function by taking moments of this equation, i.e. multiplying with the dyadic product $\underbrace{\mathbf{n} \circ \ldots \circ \mathbf{n}}_{k}$ and integrating over all orientations $\mathbf{n} \in S^2$. This set of equations is analogous to the differential equations for the alignment tensors in liquid crystal theory [19] and will be discussed elsewhere in more detail. In general the equations for the different tensor orders are coupled.

As in our model all cracks in a volume element have the same angular velocity, namely that of the surrounding material, this set of equations simplifies to a set of very special balance type equations without production, and without non-convective flux, which are not coupled:

$$(4.7) \qquad \frac{\partial a^{(k)}}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla a^{(k)} + \frac{1}{2}(\nabla \times \mathbf{v}) \cdot a^{(k)} - \frac{1}{2}a^{(k)} \cdot (\nabla \times \mathbf{v}) = 0,$$

$$(4.8) \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{or} \;\; \overset{\circ}{\mathbf{a}}^{(k)} = 0$$

for any tensor order k. This special form arises due to the model assumption of a fixed crack number and in addition cracks not moving and rotating independently of the surrounding material. Therefore for an observer co-moving with the material, the orientation distribution and the alignment-fabric tensors do not change. These equations are the equations of motion for the internal variables, which have to be postulated in a purely macroscopic theory. For our simplified crack dynamics the dynamics of the alignment-fabric tensors is not independent of the motion of the material elements. Therefore the change of the alignment tensors in time is not relevant to be considered in our simplified model, as it is completely determined by the motion of the surrounding material. However, the situation is different for other, more complicated crack dynamics. In any case, even if the dynamics of the tensorial damage parameters is not interesting, the orientation distribution itself is relevant, because of the dependence of the effective stress on crack orientation (see below). This effective stress determines the dynamics, as it appears for instance in the Griffith criterion for the onset of growth, and it also appears in the expressions for the length change velocity discussed in the examples below.

Orientation dependence of the effective stress

In an experiment with uniaxial tension σ applied to the sample the stress component σ_n, normal to the crack surface, depends on crack orientation.

Let us assume that in an experiment a uniaxial tension σ is applied along the z-direction. Then the stress component in the direction $\mathbf{n}$, acting on a crack surface with surface unit normal $\mathbf{n}$ is

$$(4.9) \qquad \sigma_{\text{eff}} = \sigma(\mathbf{e}_z \cdot \mathbf{n})^2,$$

where $\mathbf{e}_z$ is the unit vector in z-direction. This dependence of the effective stress on crack orientation leads after averaging over all orientations to

$$(4.10) \qquad \int_{S^2} \sigma_{\text{eff}} f(l, \mathbf{n}, \mathbf{x}, t) d^2 n = \int_{S^2} \sigma(\mathbf{e}_z \cdot \mathbf{n})^2 f(l, \mathbf{n}, \mathbf{x}, t) d^2 n$$

$$= \left(\int_{S^2} \sigma \left(\mathbf{nn} - \frac{1}{3}\delta \right) f(l, \mathbf{n}, \mathbf{x}, t) d^2 n + \frac{1}{3}\delta \int_{S^2} \sigma f(l, \mathbf{n}, \mathbf{x}, t) d^2 n \right) : \mathbf{e}_z \mathbf{e}_z$$

$$= \sigma \left(\mathbf{a} + \frac{1}{3}\delta \right) : \mathbf{e}_z \mathbf{e}_z = \sigma \left(a_{zz} + \frac{1}{3} \right),$$

where a_{zz} is the zz-component of the second order alignment-fabric-tensor $\mathbf{a}$. This dependence of the effective stress on the alignment-fabric-tensor leads to a dependence of the crack dynamics (for instance the critical length) on the orientational order. Thus macroscopic equations of motion of damage parameters depend on the orientational order characterized macroscopically by the alignment-fabric tensors. Hence it would be interesting to study the dynamics of the alignment-fabric-tensors, too.

4.5. Differential equation for the damage parameter

Differentiating the definition of the damage parameter equation (4.1) with respect to time we get the following differential equation for the damage parameter:

$$(4.11) \qquad \frac{dD(\mathbf{x}, t)}{dt} = \frac{d}{dt} \int_L^{l_M} \int_{S^2} f(l, \mathbf{n}, \mathbf{x}, t) d^2 n l^2 dl$$

$$= \int_L^{l_M} \int_{S^2} \left(\frac{d}{dt} f(l, \mathbf{n}, \mathbf{x}, t) l^2 + f(l, \mathbf{n}, \mathbf{x}, t) 2l\dot{l} \right) d^2 n dl$$

(4.11)
[cont.]

$$= \int_L^{l_M} \int_{S^2} \left(-\frac{\partial}{\partial l} \left(l^2 f(l, \mathbf{n}, \mathbf{x}, t) \dot{i} \right) + f(l, \mathbf{n}, \mathbf{x}, t) 2 l \dot{i} \right) d^2 n dl$$

$$= - \left[l^2 f(l, \mathbf{n}, \mathbf{x}, t) \dot{i} \right]_L^{l_M} + 2 \int_L^{l_M} \int_{S^2} f(l, \mathbf{n}, \mathbf{x}, t) l \dot{i} d^2 n dl.$$

The differential equation for the damage parameter depends on the crack distribution function itself, and therefore also on the initial crack distribution, and it also depends on the dynamical equation for the crack length.

5. Examples of closed differential equations for the distribution function

Some model on the growth velocity of a single crack is needed in order to make a closed differential equation for the length and orientation distribution function out of Eq. (3.10). Two different dynamics of crack extension from the literature will be given here as examples. In the second example we suppose that for a given load not all cracks start growing but only cracks exceeding a certain critical length l_c, which is given by the Griffith criterion. As in many examples of a crack length change dynamics, the cracks do not stop growing but extend infinitely, in all these cases the maximal crack length has to be set to $l_M = \infty$. However, when the cracks become macroscopic their growth dynamics, becomes more complicated (showing for instance branching) than our example dynamics.

5.1. Mott's extension of Griffith's energy criterion including a kinetic crack energy

When the cracks are growing the system has a kinetic energy due to the growth by virtue of the inertia of the material surrounding the separating crack surfaces. This extension of the original Griffith energy concept (see below) by a kinetic energy term goes back to MOTT [29]: A kinetic energy term is added to the sum of the crack surface energy and the elastic deformation energy of the surrounding elastic material, and the crack length is such that the total energy of the system is constant. Two different loading conditions are especially interesting: fixed loading ("dead weight") and "fixed grips" conditions. In both experiments uniaxial symmetry is assumed. In the first case a constant force is applied to the ends of the specimen, leading to a tensile stress. In the second case a fixed displacement is prescribed at the outer boundaries of the specimen. For these two loading conditions, requiring a constant total energy and an argument based on geometrical similarity, the following expressions for the crack length change velocity have been derived ([30] p. 93):

"Dead weight":

$$(5.1) \qquad \dot{l} = \dot{l}_T \left(1 - \frac{l_0}{l} \right),$$

where $\dot{l}_T$ is the so-called terminal velocity, not depending on the crack length, but on the applied load σ_{eff}, and therefore on crack orientation. l_0 is the initial crack length.

"Fixed grips":

$$(5.2) \qquad \dot{l} = \dot{l}_T \left(1 - \frac{l_0}{l} \left(2 - \frac{l_0}{l} \right) \left(\frac{1 + \alpha \dfrac{l^2}{l_0^2}}{(1 + \alpha)^2} \right)^{1/2} \right),$$

where the parameter α is defined as

$$(5.3) \qquad \alpha = \frac{8\pi l_0^2}{A}.$$

It is the ratio of the initial crack area to the surface area A of a cross-section of the specimen. In the "fixed grips" geometry the crack extension might stop again after a certain growth. This can be understood, because of the increase in compliance associated with crack extension in a finite specimen. This leads to a diminishing applied force and decreasing tendency of the crack growth.

From the mesoscopic point of view the growth laws, Eqs. (5.2) as well as (5.1) are mesoscopic constitutive equations relating the length growth velocity $\dot{l}$ to the external load in a material-dependent manner.

In both loading conditions discussed here the crack velocities have been derived for single cracks. If we apply these growth velocities in our differential equation for the length distribution function, Eq. (3.10), this means that we neglect interaction between cracks. However, crack interactions can be taken into account by more sophisticated expressions for the length change velocity.

Inserting the length change velocities of the previous section into the differential equation for the crack distribution function, and integrating over all orientations leads to the following closed differential equations:

"Dead weight":

$$(5.4) \qquad \frac{df(l, \mathbf{x}, t)}{dt} = -\frac{1}{l^2} \frac{\partial}{\partial l} \left(l^2 f(l, \mathbf{x}, t) \dot{l}_T \left(1 - \frac{l_0}{l} \right) \right).$$

The parameter $\dot{l}_T$ depends on the effective load σ_{eff} and therefore on the second order alignment-fabric tensor.

"Fixed grips":

$$(5.5) \qquad \frac{df(l, \mathbf{x}, t)}{dt} = -\frac{1}{l^2} \frac{\partial}{\partial l} \left(l^2 f(l, \mathbf{x}, t) \dot{l}_T \left(1 - \frac{l_0}{l} \left(2 - \frac{l_0}{l} \right) \left(\frac{1 + \alpha \frac{l^2}{l_0^2}}{(1+\alpha)^2} \right) \right)^{1/2} \right),$$

5.2. Griffith criterion for the onset of growth

The criterion for the cracks to start growing adopted in the example is the energy criterion introduced originally by GRIFFITH [31]. According to GRIFFITH [31] there is a criticality condition for the crack growth to start, and for cracks larger than a critical length there is a velocity of crack growth $\dot{l}$. From energetic considerations GRIFFITH [31] derived a critical length of cracks with cracks exceeding this length starting to grow. This critical length is given by:

$$(5.6) \qquad l_c = \frac{K}{\sigma_n^2},$$

where K is a material constant, and σ_n is the stress applied perpendicularly to the crack surface. It is assumed that a stress component within the crack plane does not cause the crack growth. For cracks smaller than the critical length l_c the energy necessary to create the crack surface exceeds the energy gain due to release of stresses.

5.3. Rice–Griffith dynamics

A possible crack dynamics, taking into account the criticality condition of Griffith, is derived from a generalization of the Griffith energy criterion on thermodynamic grounds, introducing the Gibbs potential [32], which includes the stress normal to the crack surface and crack length as variables. The resulting crack evolution law has the form

$$(5.7) \qquad \dot{l} = -\alpha + \beta \sigma^2 l \qquad \text{for} \quad l \geq l_c,$$

$$(5.8) \qquad \dot{l} = 0 \qquad \text{for} \quad l < l_c$$

with material coefficients α, and β. In case of a constant time rate of the applied stress, $\sigma = v_\sigma t$, it results:

$$(5.9) \qquad \dot{l} = -\alpha + \beta v_\sigma^2 l t^2 \qquad \text{for} \quad l \geq l_c,$$

$$(5.10) \qquad \dot{l} = 0 \qquad \text{for} \quad l < l_c.$$

v_σ is the time derivative of the applied stress normal to the crack surface. The dependence of this normal stress on crack orientation leads to the following orientation dependence of the dynamics:

$$(5.11) \qquad \dot{l} = -\alpha + \beta v_{\sigma\,0}^2 l t^2 (\mathbf{e}_z \cdot \mathbf{n})^4 \quad \text{for} \quad l \geq l_c,$$

$$(5.12) \qquad \dot{l} = 0 \qquad \text{for} \quad l < l_c,$$

where $v_{\sigma\,0}$ is the change velocity of the stress applied in the z-direction.

After averaging over all orientations, this orientation dependence leads to a dependence on the fourth moment $\int_{S^2} \mathbf{nnnn} f d^2 n$ of the distribution function.

This dynamics also includes a criticality condition for the crack to start growing.

With this model for the length change velocity we end up with the following differential equation for the distribution function:

$$(5.13) \qquad \frac{df(l, \mathbf{n}, \mathbf{x}, t)}{dt} = -\frac{1}{l^2} \frac{\partial}{\partial l} \left(l^2 \left(-\alpha + \beta v_\sigma(\mathbf{n})^2 l t^2 \right) \right) \qquad \text{for} \quad l \geq l_c,$$

$$(5.14) \qquad \frac{df(l, \mathbf{n}, \mathbf{x}, t)}{dt} = 0 \qquad \text{for} \quad l < l_c.$$

Solutions of this differential equation are discussed in [27].

6. Conclusions

In the mesoscopic description we have introduced mesoscopic fields, defined on an enlarged space including crack size and orientation. Averages over crack sizes and orientations, i.e. macroscopic quantities are calculated with a distribution function f. The differential equation for this distribution function was derived from the mesoscopic balance equations and crack growth law for the single crack. Different crack growth laws from the literature were discussed.

Macroscopic quantities accounting for the progressive damage have been defined as integrals calculated with the distribution function. These are scalar damage parameters, like for instance the average crack length, and fabric-alignment tensors. For these different scalar and tensorial damage parameters equations of

motion have been derived. The time evolution of fabric-alignment tensors will be of special importance under biaxial loading conditions.

The equations of motion for the damage parameters can be compared to the evolution equation in phase field models (or in Landau theory of phase transitions). In phase field models an additional wanted field, the phase field is introduced. The form of the equation of motion, often in the form of a conservation law is postulated [33, 34]. This phase field can be compared to the damage parameter introduced here, and in the non-unilateral case also to the fabric-alignment-tensor. The equation of motion for the damage parameter is of the same type. It is a special form of a balance equation, here with a zero flux term, because spatial inhomogeneities were not taken into account. However, this form of equation of motion has not been postulated here, but derived from mesoscopic considerations, i.e. mesoscopic balance equations.

Acknowledgments

References

1. W. MUSCHIK, *Internal variables in non-equilibrium thermodynamics*, J. Non-Equilib. Thermodyn., **15**, 1990.

2. G. A. MAUGIN and W. MUSCHIK, *Thermodynamics with internal variables*, J. Non-Equilib. Thermodyn., **19**, 1994.

3. L. M. KACHANOV, *On the time to failure under creep conditions*, Izv. AN SSSR, Otd. Tekhn. Nauk., 8, 1958.

4. G. A. MAUGIN, *The Thermomechanics of Plasticity and Fracture*, Chap. 7, Cambridge University Press, Cambridge 1992.

5. D. KRAJCINOVIC, *Damage mechanics*, Elsevier, Amsterdam, etc., 1996.

6. K. I. KANATANI, *Distribution of directional data and fabric tensors*, International Journal of Engineering Science, **22**, 2, 149–164, 1984.

7. J. L. ERICKSEN, *Anisotropic fluids*, Arch. Rat. Mech. Anal., 4, 1960.

8. F. J. LESLIE, *Some constitutive equations for liquid crystals*, Arch. Rat. Mech. Anal., 28, 1965.

9. S. HESS, *Irreversible thermodynamics of nonequilibrium alignment phenomena in molecular liquids and in liquid crystals*, Z. Naturforsch., **30a**, 728–733, 1975.

10. G. A. Maugin and R. Drouot, *Thermodynamic modelling of polymers in solution*, [in:] Axelrad and W. Muschik [Eds.], Constitutive Laws and Microstructure, Springer Verlag, 1988.

11. E. A. Brener, H. Müller-Krumbhaar and R. Spatschek, *Coarsening of cracks in a uniaxially strained solid*, Phys. Rev. Let., **86**, 7, 1291–1294, 2001.

12. Z. P. Bažant and D. Novák, *Probabilistic nonlocal theory for quasibrittle fracture initiation and size effect. i: theory*, J. Eng. Mech., **126**, 2, 166–174, 2000.

13. S. Gluzman and D. Sornette, *Self-consistent theory of rupture by progressive diffuse damage*, Physical Review E, **63**, 6, 066129, 11, 2001.

14. J. V. Andersen, D. Sornette and K. Leung, *Tricritical behaviour in rupture induced by disorder*, Physical Review Letters, **78**, 11, 2140–2143, 1997.

15. R. L. Blumberg Selinger, Yhang-Gang Wang, W. Gelbart and A. Ben-Shaul, *Statistical-themodynamic approach to fracture*, Physical Review A, **43**, 8, 4396–4400, 1991.

16. S. Zapperi, P. Ray, H. E. Stanley and A. Vespignani, *First-order transition in the breakdown of disordered media*, Physical Review Letters, **7**, 8, 1408–1411, 1997.

17. S. Zapperi, P. Ray, H. E. Stanley and A. Vespignani, *Avalanches in breakdown and fracture processes*, Physical Review E, **59**, 5, 5049–5057, 1999.

18. P. Van, C. Papenfuss and W. Muschik, *Mesoscopic dynamics of microcracks*, Physical Review E, **62**, 5, 6206–6215, 2000.

19. S. Blenk, H. Ehrentraut, and W. Muschik, *Statistical foundation of macroscopic balances for liquid crystals in alignment tensor formulation*, Physica A, **174**, 119–138, 1991.

20. S. Blenk, H. Ehrentraut, and W. Muschik, *Orientation balances for liquid crystals and their representation by alignment tensors*, Mol. Cryst. Liqu. Cryst., **204**, 133–141, 1991.

21. C. Papenfuss, *Theory of liquid crystals as an example of mesoscopic continuum mechanics*, Computational Materials Science, **19**, 45–52, 2000.

22. H. Ehrentraut, *A unified mesoscopic continuum theory of uniaxial and biaxial liquid crystals*, Wissenschaft und Technik Verlag, Berlin 1996.

23. H. Ehrentraut, W. Muschik, and C. Papenfuss, *Mesoscopically derived orientation dynamics of liquid crystals*, J. Non-Equilib. Thermodyn., **22**, 285–298, 1997.

24. W. Muschik, *An amendment to the second law of thermodynamics*, J. Non-Equilib. Thermodyn., **21**, 175–192, 1996.

25. S. Blenk, H. Ehrentraut, and W. Muschik, *Macroscopic constitutive equations for liquid crystals induced by their mesoscopic orientation distribution*, Int. J. Engng. Sci., **30**, 9, 1127–1143, 1992.

26. S. Blenk and W. Muschik, *Mesoscopic concepts for constitutive equations of nematic liquid crystals in alignment tensor formulation*, ZAMM, **73**, 4–5, T331–T333, 1993.

27. P. Ván, C. Papenfuss, and W. Muschik, *Griffith cracks in the mesoscopic micocrack theory*, published online, Condensed Matter, abstract, cond-mat/0211207; sent to Phys. Rev. E, 2002.

28. H. EHRENTRAUT and W. MUSCHIK, *On symmetric irreducible tensors in d-dimensions,* ARI, 51, 1998.

29. N. F. MOTT, *Brittle fracture in mild steel plates,* Engineering, 165, 1948.

30. B. LAWN. *Fracture of brittle solids,* Cambridge University Press, Cambridge 1993.

31. A. A. GRIFFITH, *The theory of rupture,* Trans. First Intl. Cong. Appl. Mech., Delft 1924.

32. P. VÁN. *Internal thermodynamic variables and failure of microcracked materials,* J. Non-Equilib. Thermodyn., **26**, 2, 167–189, 2001.

33. O. PENROSE and P. C. FIFE, *Thermodynamically consistent models of phase-field type for the kinetics of phase transitions,* Physica D, **43**, 44–62, 1990.

34. L. O. EASTGATE, J. P. SETHNA, M. RAUSCHER, T. CRETEGNY, C. S. CHEN, and C. R. MYERS, *Fracture in mode i using a conserved phase-field model,* Phys. Rev. E, **65**, 3, 2002.