Internal thermodynamic variables and failure of microcracked materials

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Abstract

Thermodynamic stability of materials is investigated in the presence of internal variables. The possibility of phase boundaries in nonequilibrium solid materials is considered which suggests the concept of *phase breaking* similar to the phase transitions in case of fluid and gaseous systems. Two particular models of damage mechanics are proposed and investigated in more detail as illustrative examples. Both models are direct thermodynamic generalizations of well known damage mechanical models considering general loading conditions. According to these thermodynamic suggestions a new failure criterion is suggested for microcracked materials and compared with experiments and other criteria.

1 Introduction

Discussing the mechanical properties of materials (brittle, quasi-brittle and ductile) we can distinguish between two kinds of theories. There are theories for the failure (yield) dealing with the strength of different materials and there are theories that give the change of mechanical properties under different loading conditions. The two kinds of models appear separately. The models in the first group, the damage motivated *failure theories* do not say anything about the change of mechanical properties (e.g. stiffness) of materials. The classical energy condition of Griffith gives an example. The second group contains most of the *rheological models* for ductile or *damage mechanical* models for brittle materials. Some damage mechanical theories can give more information, one of their appealing properties is that an increasing damage leads to failure therefore a damage theory can result in a failure/fracture criteria at the same time. Unfortunately this is rather an exception than a rule, most of the damage theories introduce the critical damage ad hoc, giving a single critical value or a whole "damage surface" for different loading conditions.

The problem is that the mechanical properties of real materials, the experimental facts show confusing complexity. One can meet a lot of connected and frequently parallel phenomena. Brittle-ductile transitions, localization, different microstructural effects are the most important aspects that a damage theory should take into account. On the other hand, materials with different microstructure and different microscopic damage processes can show similar stress-strain relations in experiments and in micromechanical-statistical models (see for example the investigations of Kemeny and Cook [1]). Therefore the microscopic details seem to be negligible and we can hope a unified damage-failure theory on the base of phenomenological thermodynamic principles.

The thermodynamic models for describing the mechanical properties of materials and the change of the microstructure introduce *internal thermodynamic variables* of different tensorial order. Recently several thermodynamic models were proposed for brittle and quasi-brittle microcracked materials (see e.g. in

[2, 3]). According to these investigations we can see that continuum damage mechanics is able to produce a fitting of experiments in a lot of details but the price we pay is that failure appears as an external condition to be measured. Equilibrium thermodynamics suggests a well defined mechanism to deal with material instabilities: the notion of phases and phase transitions. Failure is a kind of material instability. To give a possible description of the connection of damage and failure we investigate whether we could extend the usual equilibrium thermodynamic formalism to nonequilibrium theories with internal variables.

2 Internal variables and stability: thermodynamic requirements

It is well known that the Second Law expresses a stability requirement for materials. There are two different aspects to be considered:

- *Thermodynamic stability*; the convexity of entropy function. This is a static stability requirement that ensures the stability of equilibrium states of matter in case of external perturbations of the thermodynamic state, independently of the particular dynamic equations. Phase boundaries appear where thermodynamic stability is violated.
- *Dynamic stability* of thermodynamic equilibrium; positive entropy production, where a particular dynamic equation of matter is considered. The connection between the two stability concepts is clear, both thermodynamic and dynamic stability restrict the possible functional form of the constitutive functions to give together the asymptotic stability of thermodynamic equilibrium [4, 5]. For homogeneous (discrete) systems this idea was developed in detail giving a remarkable conceptual background of the Second Law [6, 7, 8, 9].

Now, in this paper this stability point of view of thermodynamics gives the key to the understanding of the proposed frame for the unified treatment of fracture and failure of brittle materials.

In the last decades the theory of internal variables has been an important contribution to equilibrium and irreversible thermodynamics. This is a relatively simple way to treat phenomenological thermodynamic systems out of local equilibrium. Several kinds of internal variables are introduced in the literature under different names depending on what properties of the equilibrium variables are preserved and extended. As a simplest classification we distinguish between internal variables describing the *history dependence* (see Coleman and Gurtin [10]) and internal variables related to neighborhood sensitivity, *nonlocality* of equilibrium state variables (see e.g. [11]). Here in the following we use internal variables in the first sense (history dependence), and we require that they should vanish in local equilibrium [12]. Several special theories with a lot of applications were developed using this concept. For example, in the so called "extended thermodynamic" theories Onsagerian currents are introduced as internal variables. However, the success of thermodynamic theory of metal plasticity shows an example that the applicability of internal variables is beyond extended thermodynamics [13].

The early, ad-hoc applications of internal variables to explain some experimental anomalies introduced additional terms into the governing equations (resulting e.g. in the Cattaneo-Vernotte heat conduction, etc..) but later a general thermodynamic frame was developed to make the dynamic equations compatible with the Second Law. The key revelation in this unification was a kind of canonical representation starting from the following separation of the entropy function into an equilibrium and non-equilibrium part

$$S(\mathbf{x}_e, \boldsymbol{\alpha}) = S_e(\mathbf{x}_e) - \frac{1}{2}\sum_{j=1}^{N} m_j(\alpha_j)^2, \tag{1}$$

where the vector $\mathbf{x}_e = (x_{ei})$, $i = 1, ..., n$ of classical equilibrium variables form the *equilibrium state space* which together with the vector $\boldsymbol{\alpha} = (\alpha_j)$, $j = 1, ..., N$ of internal variables constitute the *nonequilibrium state space.* The positive or positive definite quantities $\boldsymbol{m} = (m_j)$, $j = 1, ..., N$ are the *thermodynamic inductivities.* The above form of the entropy function was introduced by Gyarmati [14] and has been used extensively in the literature of extended thermodynamics. This representation is based on the Second Law, the requirement that the entropy function should have a maximum at local thermodynamic equilibrium [15]. In case of fluid and gaseous phases this form of the entropy function can be supported by statistical, kinetic calculations. However, the nonequilibrium variables $\boldsymbol{\alpha}$ can be introduced in an abstract manner: due to the Morse lemma, any real physically motivated variable can be transformed in such a way that the entropy function has the form (1) in a neighborhood of local equilibrium. Unfortunately, this form of the entropy has some disadvantages:

- According to (1) the entropy function S is *globally* concave (moreover has a maximum) on the nonequilibrium part of the state space, in the internal variables $\boldsymbol{\alpha}$. However, as it was mentioned, this is an approximation, there is a neighborhood of the equilibrium state, where it is valid. This neighborhood depends on the considered transformation and can be very small.

- The nonequilibrium variables do not necessarily have a *clear physical interpretation*, the mentioned transformation in the Morse lemma can mix several physical variables.

The first point suggests some interesting questions and possibilities. If the form (1) is not global, the nonequilibrium entropy is not necessarily a convex function in the whole nonequilibrium phase space. In the equilibrium phase space the violation of the convexity means the loss of thermodynamic stability, a presence of a phase boundary. What can be a meaning of the loss of thermodynamic stability in the nonequilibrium state space? Is there a physical phenomenon which can be well described with the help of this concept?

As regards the second point, the form (1) is not the only nonequilibrium entropy function used in macroscopic physics. There are examples with more physical internal variables resulting in more complicated nonequilibrium entropy functions. For example, the classical director theory of liquid crystals is based on a different expression (see the original contributors [16, 17]).

Therefore, we may look for phenomena where a nontrivial entropy function is convex near to equilibrium, but the thermodynamic stability is violated for sufficiently large internal variable values. In the following we will see that the damage and the change of mechanical properties of brittle materials (rocks, glasses, ceramics) could give an example: simple models can be proposed where a natural, physically motivated entropy function arises. In this paper we investigate the thermodynamic stability of some particular entropy functions and compare the results with empirical strength criteria.

3 Irreversible thermodynamics of damaged materials

Solid materials can be classified by their uniaxial stress-strain curves beyond the traditional elastic regime. One of the possible classifications is to distinguish between the ideally plastic (ductile) and brittle materials (Fig 1/a,b) and their combination as for example the special quasi-brittle and ductile-brittle behavior (see Fig 1/c,d) [2]. The dashed arrows on the figures denote the characteristic unloading curves. The plasticity is characterized by the residual strain and the brittleness is explained by defects destroying the cohesion of the material. However, the interpretation of these curves with internal structural changes is not very straightforward. For example, the strong rate dependence of these relations can be an important aspect to consider. The same material can be ductile with high loading rates and brittle for slow ones and contrary. On the other hand, similar curves can cover very different internal structural changes: dislocation movements in metals, cracking in rocks and grain movements in soils can lead to the same 'plastic' behavior.

In the following we will develop an internal variable approach to deal with a group of materials (like ceramics, rocks, ...), generally considered as brittle, where the microcracks form the typical microstructural change, the damage. In this case the interpretation of the internal variables is more or less clear and it can be exploited in developing special simple models. In microcracked materials the internal defects can be idealized as penny shaped thin holes and usually are represented by their surface vectors. In general, we characterize the microstructural changes resulting in the damaged behavior with internal variables α^i, $i = 1, 2, .., N$, denoted by a single vector $\boldsymbol{\alpha} = (\alpha^i)$. Their number and tensorial order depend on the physical mechanisms to be considered and on the intended degree of approximation of the real material behavior. With the above mentioned penny shaped cracks the damage is best represented by the distribution function of the microcrack surface vectors and the related macroscopic internal variables can be the different moments of this distribution function [18, 19]. These kinds of internal variables are of averaging type, they are imagined as "smoothed out" local internal variables in space, i.e. spatial averages of local internal variables over a representative volume element (see e.g. [20]). Of course a simple average of the micro surface vectors can also be good for several purposes, like the directors in the mentioned theories of liquid crystals, with similar restrictions [21].

In any case, with these averaging type variables the conjugated 'intensive' variables, the corresponding affinities vanish at equilibrium states, in this sense they are dynamic degrees of freedom [22, 23, 12]. Moreover, a thermodynamic process can be assumed to be continuous. On the other hand, as we are dealing with internal variables representing different kinds of damage in elastic material, some or all of the introduced internal variables can be frozen. In case of some frozen internal variables the material is not in a thermodynamic equilibrium in the sense that the corresponding affinities are not zero, that is, the material is in a *constrained equilibrium*. After these preliminary considerations we can go ahead to formulate the corresponding thermodynamic frame.

3.1 Statics

We concentrate upon the mechanical properties, therefore electromagnetic, chemical, diffusive, etc. effects are excluded in our treatment. In the following all quantities and fields are defined relative to the reference configuration. First we treat the appropriate thermodynamic theory for homogeneous (discrete) materials. The static and dynamic thermodynamic requirements are strongly distinguished. This treatment can serve as a 'thermostatic' background of a continuum description, where we can say that we consider a representative volume element in the usual way: Sufficiently large in size to behave macroscopically as if it were homogeneous and sufficiently small to be treated as a point in a continuum.

The traditional equilibrium state space of the variables $\mathbf{x}_e = (s, \epsilon)$ is supplemented by the vector of internal variables $\boldsymbol{\alpha}$. The corresponding nonequilibrium state vector and state space of our mechanical system is therefore denoted as $(s, \epsilon, \boldsymbol{\alpha}) \in \mathcal{D}_u$. $\mathbf{A}(s, \epsilon, \boldsymbol{\alpha}) = (A_i(s, \epsilon, \alpha_1, ..., \alpha_N))$, $i = 1, ..., N$ will be called the affinity conjugated to $\boldsymbol{\alpha}$. The Gibbs relation can be given in our case as

$$\mathrm{d}u = T\mathrm{d}s + \mathbf{t} : \mathrm{d}\epsilon - \mathbf{A} \cdot \mathrm{d}\boldsymbol{\alpha}, \tag{2}$$

where u is the internal energy density, s is the entropy density, T is the absolute temperature, and ϵ and $\mathbf{t}$ are the deformation and the stress, respectively. As we are in the reference configuration, $\mathbf{t}$ coincides with the Cauchy stress. The colon denotes the contraction of second order tensors and the dot a similar operation with the affinities and internal variables, considering, that their tensorial properties are not specified. The assumed validity of the Gibbs relation means that the Kelvin-Planck form of the Second Law, the existence of the entropy function is applied for non-equilibrium states and processes. Regarding that our investigations are strongly related to the stability of the mechanical material, the extent and the content of this assumption is clear, moreover, as a particular example, shows the possible limits of similar extensions.

Since we are dealing with pure mechanical systems it is convenient to introduce the Helmholtz free energy density as a partial Legendre transform of the internal energy u with respect to s,

$$\phi := u - Ts = \phi(T, \epsilon, \boldsymbol{\alpha}). \tag{3}$$

The corresponding form of (2) becomes

$$\mathrm{d}\phi = -s\mathrm{d}T + \mathbf{t} : \mathrm{d}\epsilon - \mathbf{A} \cdot \mathrm{d}\boldsymbol{\alpha}. \tag{4}$$

Therefore the partial differentials are

$$s = -\frac{\partial \phi}{\partial T}, \qquad \mathbf{t} = \frac{\partial \phi}{\partial \epsilon}, \qquad \mathbf{A} = -\frac{\partial \phi}{\partial \boldsymbol{\alpha}} \tag{5}$$

and the corresponding state vector in the state space is denoted by $(T, \epsilon, \boldsymbol{\alpha}) \in \mathcal{D}_\phi$.

Finally a third thermodynamic potential is introduced, the Gibbs free energy as a partial Legendre transform of ϕ with respect to ϵ

$$\psi := \phi - \mathbf{t} : \epsilon = \psi(T, \mathbf{t}, \boldsymbol{\alpha}). \tag{6}$$

The corresponding form of the Gibbs relation follows

$$\mathrm{d}\psi = -s\mathrm{d}T - \epsilon : \mathrm{d}\mathbf{t} - \mathbf{A} \cdot \mathrm{d}\boldsymbol{\alpha}. \tag{7}$$

Here the state vector is $(T, \mathbf{t}, \boldsymbol{\alpha}) \in \mathcal{D}_\psi$ and the partial derivatives are

$$s = -\frac{\partial \psi}{\partial T}, \qquad \epsilon = -\frac{\partial \psi}{\partial \mathbf{t}}, \qquad \mathbf{A} = -\frac{\partial \psi}{\partial \boldsymbol{\alpha}}. \tag{8}$$

Sometimes this state space and the Gibbs free energy are the most convenient to treat mechanical problems.

3.2 Thermodynamic stability

Only the Helmholtz and Gibbs free energy representations are considered and the temperature is supposed to be constant (a pure mechanical problem is treated). The general requirement of thermodynamic stability states that the Helmholtz free energy should be a concave function of its variables. In case of two times differentiable free energy a material is thermodynamically stable at a given fixed temperature T with deformation ϵ and internal variable $\boldsymbol{\alpha}$, if the second derivative of the Helmholtz free energy is a positive definite function:

$$(\mathrm{d}\epsilon, \mathrm{d}\alpha) \cdot D^2\phi(\epsilon, \boldsymbol{\alpha}) \cdot (\mathrm{d}\epsilon, \mathrm{d}\boldsymbol{\alpha}) = (\mathrm{d}\epsilon, \mathrm{d}\boldsymbol{\alpha}) \cdot \begin{pmatrix} \frac{\partial^2 \phi}{\partial \epsilon^2} & \frac{\partial^2 \phi}{\partial \boldsymbol{\alpha} \partial \epsilon} \\ & \\ \frac{\partial^2 \phi}{\partial \epsilon \partial \boldsymbol{\alpha}} & \frac{\partial^2 \phi}{\partial \boldsymbol{\alpha}^2} \end{pmatrix} \cdot \begin{pmatrix} \mathrm{d}\epsilon \\ \mathrm{d}\boldsymbol{\alpha} \end{pmatrix} \geq 0 \tag{9}$$

for every $(d\epsilon, d\boldsymbol{\alpha})$. Here we applied a notation from the mechanical literature denoting by $d\epsilon$ and $d\boldsymbol{\alpha}$ arbitrary vectors from the linear spaces where the deformation ϵ and the internal variables $\boldsymbol{\alpha}$ were defined. In this sense for example $d\epsilon$ can be an arbitrary symmetric second order tensor. $D^2\phi$ denotes the derivative of ϕ with respect to its variables ϵ and $\boldsymbol{\alpha}$. In the following we will assume that the functional form of the free energy does not contain differential or integral operators. However, the process dependence of the corresponding equations is considered through the introduced internal variables. Therefore the resulted stress-strain relations will be clearly rate dependent, but a rate form notation is not necessary and could even be misleading. Let us remark here that the generality of the treatment is not restricted by this assumption. The different kinds of internal variables can give rate and gradient dependent stress-strain relations.

A (partially) convex Helmholtz free energy gives requirements for the Gibbs free energy, but these requirements cannot be expressed as a simple concavity of convexity for all variables (one can say that the Gibbs free energy is convex in the internal variables and concave in the other ones). Therefore a conversion to Helmholtz free energy can be useful for thermodynamic stability calculations.

The subset of the state space where these conditions are satisfied determines the *stability domain* of the damaged material. Outside this domain the equilibrium of the damaged material is unstable, without further constraint the sample fails. The boundary of the stability domain in the corresponding state space will be called the *damage surface*.

It is interesting to investigate the previous conditions more closely! In case of fluid or gaseous media with equilibrium state variables the stability loss indicates a phase boundary and a phase transition to an other phase. In case of damaged bodies the failure changes the properties of the material and the internal interactions (for example the cohesion vanishes and dry friction will be the dominating dissipation mechanism). However, in this case all of our previous assumptions on the homogeneous representative volume elements can become meaningless. In solid materials we cannot speak unambiguously of an other homogeneous phase after the loss of thermodynamic stability, in a continuum description the phases are immediately localized. This is best seen if we consider the above condition (9) of stability loss which can be interpreted as a generalization of the classical *Hadamard-Hill condition* of shear banding. Using purely mechanical arguments and investigating jump surfaces in the velocity field [24, 25, 26], shear banding appears in the direction $\mathbf{n}$ if

$$\det(\mathbf{n} \cdot \mathbf{C} \cdot \mathbf{n}) = 0, \tag{10}$$

where $\mathbf{C}$ is the fourth order stiffness tensor, that can be given as the partial derivative of the free energy,

$$\mathbf{C} := \frac{\partial^2 \phi}{\partial \epsilon^2}.$$

We can see that $\mathbf{C}$ is the $(1,1)$ submatrix in our general thermodynamic stability condition (9). A necessary condition of this submatrix be positive definite is the classical localization condition (10) of Hadamard and Hill. The requirement of a positive definite elastic moduli can be derived from energetic-stability considerations resulting in a more general localization condition. This general *energetic localization condition* considers shear-banding and cleavage type localization instabilities (see e.g. [2, 27]). Our condition (9) can be considered as a generalization of these classical requirements, but it is important that here the positive definity of the internal variable part is not taken as granted.

Therefore the loss of thermodynamic stability, at least in some cases, does not result in a homogeneous change in the material but indicates the appearance of some localized patterns, for example shear bands. Hence the analogy with phase transitions can be misleading so, instead of phase transitions, we can call this phenomena as *phase breaking*. This kind of localization condition is characteristic of solid materials because in fluids and gases the stiffness is a diagonal tensor (in equilibrium, neglecting the viscosity), therefore any localization phenomenon is strongly connected to the appearance of higher order space derivatives in the constitutive equations. In solid materials the two kinds of localization ('local' and 'nonlocal') can appear together. Let us remark here that in lattice models, treating microcracking as a nucleation process, this fact is not considered (see e.g. [28]). The proposed equations describing the cracking are all of a nonlocal type.

3.3 Dynamics

Let us proceed to find a proper form of the entropy production. We are treating a pure mechanical situation, consequently only the mechanical work contributes to the internal energy balance [29, 23]:

$$\dot{u} + \nabla \cdot \mathbf{q} = \mathbf{t} : \dot{\epsilon}. \tag{11}$$

Here $\mathbf{q}$ is the conductive current density of the internal energy (heat current). The dot above the quantities denotes substantial time derivative and we suppose that the deformation of the body is small. Using the balance of internal energy (11) and assuming that the entropy flux has the classical form $\mathbf{J}_s = \mathbf{q}/T$ (neglecting nonlocal effects [30]), we can obtain the density of the entropy production with the help of the Helmholtz and Gibbs free energies:

$$\begin{aligned} T\sigma_s &= \mathbf{q} \cdot \nabla \left(\frac{1}{T}\right) + \left(\mathbf{t} - \frac{\partial \phi}{\partial \epsilon}\right) : \dot{\epsilon} - \frac{\partial \phi}{\partial \boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} = \\ &= \mathbf{q} \cdot \nabla \left(\frac{1}{T}\right) + \left(\frac{\partial^2 \psi}{\partial \mathbf{t}^2}\right)^{-1} \left(\epsilon + \frac{\partial \psi}{\partial \mathbf{t}}\right) : \dot{\epsilon} - \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} \geq 0. \end{aligned} \tag{12}$$

It is easy to identify the thermodynamic currents and forces in the expression above. In the following we will treat isothermal processes and a uniform temperature is supposed in the solid, therefore the first term in (12) will be missing. In case of brittle solids, assuming a local mechanical equilibrium means a zero thermodynamic force for the mechanical interaction, that is why we will suppose that the viscous stresses are zero, too. The entropy production density then reduces to

$$T\sigma_s = \mathbf{t} \cdot \dot{\epsilon} - \dot{\phi} - s\dot{T} = \mathbf{A} \cdot \dot{\boldsymbol{\alpha}} \geq 0. \tag{13}$$

This inequality of the second law imposes a condition on the evolution equations for internal variables which can be assumed in the form

$$\dot{\boldsymbol{\alpha}} = f_\mathfrak{i}(\mathbf{A}, \mathbf{x}_\mathfrak{i}), \tag{14}$$

where $\mathbf{x}_\mathfrak{i}$, $\mathfrak{i} = u, \psi, \phi$ is an element of the corresponding state space. The other prescriptions and physical requirements imposed on the dynamics are included in the further properties of $f_\mathfrak{i}$.

The first property of f_i is that in case of small stresses there is an *elastic domain* $\mathfrak{E}_\mathfrak{i}$ in the $\boldsymbol{i}$ state space of the solid material in which the stress strain relations of our sample are ideally elastic and changes in $\boldsymbol{\alpha}$ are responsible for the anelastic strain, thus

$$f_\mathfrak{i}(\mathbf{A}, \mathbf{x}_\mathfrak{i}) = 0, \qquad \text{if} \quad \mathbf{x}_\mathfrak{i} \in \mathfrak{E}_\mathfrak{i}. \tag{15}$$

The condition above defines the elastic domain as a part of the state space where all the internal variables are frozen. Naturally, we can consider more general situations where only some of the internal variables are frozen, defining separate elastic domains of the different variables. The elastic domains above given in a particular state space can be transformed into each other. The boundary of $\mathfrak{E}_\mathfrak{i}$, denoted by $\partial\mathfrak{E}_\mathfrak{i}$, will be called *damage initiation surface*, inside this boundary the internal variables are frozen, outside they can evolve.

The second property of f_i comes from the requirement that a zero affinity $\mathbf{A}$ implies zero changes in $\boldsymbol{\alpha}$, i. e.

$$f_\mathfrak{i}(\mathbf{0}, \mathbf{x}_\mathfrak{i}) = 0. \tag{16}$$

We call attention to that, however $f_\mathfrak{i}(\mathbf{0}, \mathbf{x}_\mathfrak{i}) = 0$ does not imply $\mathbf{A} = \mathbf{0}$. Only the equilibrium where $\mathbf{A} = 0$ are to be considered as true thermodynamic equilibrium states. When $\mathbf{A} \neq 0$ there is a force toward the thermodynamic equilibrium, but some kinematic, 'freezing' constrains can keep the material in a 'prestressed' state. In the following we will give an example of this kind of particular kinematic freezing condition for damage processes.

The previous two conditions (15) and (16) together with the third one imposed by the Second Law (13) results in a simple linear Onsagerian approximation of the dynamic equation. Using the Lagrange mean value theorem we can write in general

$$\dot{\boldsymbol{\alpha}} = L(\mathbf{x})\mathbf{A}(\mathbf{x}). \tag{17}$$

Let us emphasize again that we developed a linear approximation around the thermodynamic equilibrium state and not around the instantaneous kinematic equilibrium, characterized by the frozen internal variables. On the other hand, we can use the full nonlinear general dynamic equation (14) keeping in mind the restrictions from the Second Law (13) the *freezing* and the *equilibrium conditions* (15) and (16).

4 The simplest models of microcracked damage

Up to this point we followed a treatment like the traditional thermodynamic theories of plasticity. However, in (metal) plasticity internal variables represent dislocation movements and some other kind of dissipative changes in the internal structure that are more or less similar to dry friction. In case of a microcracking induced damage, the internal processes are different. Cracks are opening and closing and this mechanism has some specific features that we should consider. For modeling purposes it is convenient, as a first step, to neglect friction. Though in real materials the two different (frictional and opening) mechanisms can work together, sometimes they are hardly distinguishable, there are no ideal microcracked materials without some friction.

In the following we will investigate a simple model of microcracking, introducing a single damage variable. Microcracking damage is essentially a three dimensional phenomena, therefore the simplest representation of the damage can be a single damage vector $\mathbf{D}$. For idealized penny shaped microcracks this internal variable can be interpreted as the average of the microcrack vectors in a representative volume element. Therefore the damage vector is an axial vector, whose direction is not but only its orientation is important. Naturally, a single vectorial, average type internal variable is a simplification, and the most important limit of its applicability is, that it cannot take into account separately growing damage in different directions. However, with simple loading histories (e.g. one or two axes loading) we can expect that our model will be in a good agreement with the experiments. More internal variables with higher tensorial orders or the whole distribution function as a variable could give better, but more complicated models. As we mentioned previously, the situation is similar to liquid crystals, where the macroscopic director theory of Ericksen-Leslie-Parody-Verhás gives a good description in situations near to a totally aligned state of liquid crystal molecules [21].

An important characteristic experimental property of microcracked materials is the so called *Kaiser effect.* The noises attributed to the extending microcracks can be detected in a preloaded sample when the reloading arrives at the previously applied highest stress level. This is observed in several directions separately. For some special brittle materials, e.g. rocks, it can be used to discover the loading history (the formerly applied peak stresses) [31]. This effect and the typical stress-strain relations (reloading gives an approximate linear behavior, see Fig 1) can be explained assuming that under normal environmental conditions a crack cannot heal, or at least the healing capability of the cracks is restricted [32, 33]. Of course, with higher temperatures or in extremely clear environments the microcrack extension is reversible and the Kaiser effect disappears. In the following we will investigate the ideal case of totally irreversible, non-healing cracks. From a thermodynamic point of view the Kaiser effect is a typical manifestation of frozen internal variables. Moreover, in this case we can give an explicit damage initiation condition. Namely, it is reasonable to assume that an increasing stress makes the damage grow, therefore a straightforward explanation of the Kaiser effect is that the size of the cracks can only grow,

$$\frac{\mathrm{d}}{\mathrm{dt}}(\mathbf{D}\cdot\mathbf{D}) = 2\mathbf{D}\cdot\dot{\mathbf{D}} \geq 0 \tag{18}$$

From a thermodynamic point of view (18) means an inherent irreversibility of the microfracturing process, as a result of chemical reactions on the crack surfaces. Those processes are usually on a different time scale, therefore their detailed investigation beyond the requirement (18) is not included in this treatment. If we consider the length and the orientation of $\mathbf{D}$ as separate internal variables, then the size of the cracks is a kind of unilateral thermodynamic variable [34]. On the other hand, condition (18) together with the dynamic equation (14) (or (17)) determine whether our dynamic variable $\mathbf{D}$ is frozen or not. The elastic domain in a free energy state space can be given as

$$\mathfrak{E}_\phi(T,\mathbf{D}) = \{(T,\epsilon,\mathbf{D})|\mathbf{D}\cdot f_\phi(T,\epsilon,\mathbf{D}) \leq 0\}.$$

The damage initiation surface $\partial\mathfrak{E}_\phi$ is the boundary of the set $\mathfrak{E}_\phi$. Therefore the full dynamics including the elastic domain can be given as:

$$\dot{\mathbf{D}} = \begin{cases} f_\phi(T,\epsilon,\mathbf{D}), & \text{if} \quad \mathbf{D}\cdot f_\phi(T,\epsilon,\mathbf{D}) \geq 0 \\ 0, & \text{otherwise.} \end{cases} \tag{19}$$

To arrive at an applicable thermodynamic model of microcracking, the crucial point is to give a reasonable form of the entropy (free energy) function. We can find several suggestions in the literature. The energy condition of Griffith can be considered as the first example [35]. The proper thermodynamic frame interpreting the energetic stability considerations of Griffith was given later by Rice [33]. For uniaxial loading conditions (mostly for tensile loading) several other particular forms were derived [36, 37, 38]. All of these suggestions want to preserve the original Griffith condition as a special case. Another group of free energy functions was suggested to take into account an anisotropic damage evolution. For example, using general representation principles, several models were proposed with a single vectorial internal variable, too [39, 40, 41]. We can find examples also for direct generalizations of the one dimensional models of Rabotnov and Kachanov [42, 43]. These models are particularly attractive, because they contain an inherent built in instability (supposing the $1/(1-D)$ form of the compliance) and at the same time the canonical form of the nonequilibrium entropy (1) is preserved. It is remarkable that all suggestions suppose an interaction between the equilibrium mechanical variables (strain or stress) and the introduced internal variables: in the Helmholtz (or Gibbs) free energy the two kinds of variables are not separated any more.

In the following we suggest a specific Helmholtz free energy and a Gibbs free energy based on representation theorems and we will see that, without any other assumptions, this general form can result in a thermodynamic instability with increasing damage. We will investigate the most general second order polynomial approximation of the free energy and the Gibbs function for isotropic materials in both cases. The two forms are not equivalent at all, but both have some appealing properties.

4.1 Model I. *(Helmholtz free energy representation)*

The second order polynomial approximation of the specific free energy ϕ at constant temperature according to the representation theorems of Pipkin and Rivlin [44] is

$$\begin{aligned}
\phi(\epsilon, \mathbf{D}) &= (\delta + k_\delta \mathbf{D}^2)\mathrm{Tr}\epsilon + (\mu + \frac{k_\mu}{2}\mathbf{D}^2)\epsilon : \epsilon + \frac{1}{2}(\lambda + k_\lambda \mathbf{D}^2)(\mathrm{Tr}\epsilon)^2 + \\
&+ \frac{\alpha}{2}\mathbf{D}^2 + \frac{1}{2}(\beta + k_\beta \mathrm{Tr}\epsilon)\mathbf{D}\cdot\epsilon\cdot\mathbf{D} + \frac{\gamma}{2}\mathbf{D}\cdot\epsilon\cdot\epsilon\cdot\mathbf{D}. \qquad (20)
\end{aligned}$$

Due to the isotropy, only ten material parameters appeared in our expression which is an extension of the free energy of purely elastic isotropic solids. The above expression gives a free energy for general loading conditions, moreover it does not contain specifications on the considered dissipation mechanism. The number of new material parameters can be reduced by physical (micromechanical) assumptions and calculations. Moreover, all terms in the expression can be interpreted from a physical point of view:

- The first term is related to the hydrostatic energy conservation of the material. δ characterizes the damage independent and k_δ the damage dependent part. Pore fluid pressure can be a physical mechanism in the background. (All of the material parameters can depend on temperature and density of the material.)
- The next two terms are the usual elastic free energy contributions where μ and λ are the well known Lamè coefficients. k_μ and k_λ characterize their damage dependence.
- The fourth term represents the energy attributed directly to the cracks.
- $\mathbf{D}\cdot\epsilon\cdot\mathbf{D}$ is the deformation at the direction of the crack surface, therefore the fifth term considers the opening of the cracks.
- The last term contains the square of the substantial crack vector change $\mathbf{D}\cdot\epsilon$, therefore it means an energy contribution necessary for turning the cracks with the deforming media.

Another clue to the interpretation of the material parameters can be given by the equation of the mechanical equilibrium (the second formula of (5))

$$\begin{aligned}
\mathbf{t} &= (\delta + k_\delta \mathbf{D}^2)I + (2\mu + k_\mu \mathbf{D}^2)\epsilon + (\lambda + k_\lambda \mathbf{D}^2)Tr\epsilon I + \qquad (21)\\
&+(\beta + k_\beta Tr\epsilon)\mathbf{D}\circ\mathbf{D} + k_\beta \mathbf{D}\cdot\epsilon\cdot\mathbf{D}I + \frac{\gamma}{2}(\mathbf{D}\circ\epsilon\cdot\mathbf{D} + \mathbf{D}\cdot\epsilon\circ\mathbf{D}).
\end{aligned}$$

where I is the unit tensor and $\circ$ is the usual notation of the tensorial product in continuum physics. Let us observe that having a linear equation, we can easily introduce a kind of plastic strain, solving the above equation for the deformation ϵ with zero stress (since we want to attach the word 'plastic' to some specific internal mechanism, a nomination *damage strain* is more appropriate). To find it we should first define a 'damage (plastic) stress' $\mathbf{t}_0$ belonging to zero deformation as

$$\mathbf{t}_0(\mathbf{D}) := \mathbf{t}(0, \mathbf{D}) = (\delta + k_\delta \mathbf{D}^2) I + \beta \mathbf{D} \circ \mathbf{D}.$$

This equation immediately gives a meaning and suggests measurement methods for the parameters δ, k_δ and β. With the damage stress the fourth order stiffness tensor $\mathbf{C}$ is given by the relation

$$\mathbf{t}(\epsilon, \mathbf{D}) = \mathbf{t}_0(\mathbf{D}) + \mathbf{C}(\mathbf{D}) \cdot \epsilon,$$

therefore, the *damage strain* $\epsilon_0(\mathbf{D})$ will be

$$\epsilon_0(\mathbf{D}) = -\mathbf{C}^{-1}(\mathbf{D}) \mathbf{t}_0(\mathbf{D}).$$

Moreover, equation (21) of the mechanical equilibrium shows well that the suggested free energy function can be considered as a direct generalization of the idea of the classical Kachanov-Rabotnov theory (where the damage can be connected to the reduction of the effective load carrying area) (see e.g. [45]). In this case, in every direction $\mathbf{n}$, a second order damage tensor $\mathcal{D}_\mathbf{n}$ can be introduced with the help of the stiffness as $\mathbf{n} \cdot \mathbf{C} \cdot \mathbf{n} = I - \mathcal{D}_\mathbf{n}$. A detailed interpretation of the damage in this direction is given in [42, 43].

One of the advantages of our internal variable model is that we can give explicitly the thermodynamic stability threshold (9) (therefore the Hadamard-Hill localization condition, too). Calculating (9) from (20), our first observation is that there are no values of the material parameters that would result in a stable material for *any* strain and damage. Some particular necessary conditions for the positive definiteness of the matrix (9) can be calculated easily.

1. In case of zero damage the convexity of the free energy is ensured by the well known sign restrictions of Lamè coefficients

   $$\mu > 0 \qquad \text{and} \qquad \mu + \lambda > 0.$$

2. When the deformation is zero, we get

   $$\alpha > 0.$$

3. General simple results cannot be derived, but in two dimensions and in case of some specific conditions for the material coefficients we get upper limits for the length of the damage:

   - If $2k_\mu + k_\lambda + k_\beta + \lambda/2 < 0$ then

     $$-\frac{2\mu + \lambda}{2k_\mu + k_\lambda + k_\beta + \lambda/2} > \mathbf{D}^2$$

– If $4k_\mu + \gamma < 0$ then

$$-\frac{4\mu}{4k_\mu + \gamma} > \mathbf{D}^2$$

The thermodynamic stability is violated, the material fails if the length of the damage arrives at these limits.

These inequalities restrict the possible values of the material coefficients and what is more important, they give material dependent upper limits on the possible damage values. Let us observe that the damage criterion itself depends on the material. Contrary to the Kachanov-Rabotnov damage representation, we obtained two different upper limits for $\mathbf{D}^2$.

The second part of the entropy production (12) yields a detailed form of the mentioned evolution equation of the damage (17) in the first linear thermodynamic approximation, as

$$\begin{aligned} \dot{\mathbf{D}} &= \mathbf{L} \cdot \big(\alpha + 2k_\mu \epsilon : \epsilon + k_\lambda (\mathrm{Tr}\epsilon)^2 + 2k_\delta \mathrm{Tr}\epsilon)\mathbf{D} + \\ &+ 2(\beta + k_\beta \mathrm{Tr}\epsilon)\mathbf{D} \cdot \epsilon + \frac{\gamma}{2}(\epsilon \cdot \epsilon \cdot \mathbf{D} + \mathbf{D} \cdot \epsilon \cdot \epsilon\big) =: f_\phi(\epsilon, \mathbf{D}), \end{aligned} \tag{22}$$

where $\mathbf{L}$ is the symmetric second order Onsagerian conductivity tensor. In isotropic materials it has a simple form: $\mathbf{L} = lI$, where l is positive because of the Second Law.

From the equation (21) of the mechanical equilibrium we can get the deformation as the function of stress and damage $\epsilon = \epsilon(\mathbf{t}, \mathbf{D})$. Introducing these relations into the differential equation (22), we will get an equation for the evolution of the damage containing the stresses as parameters:

$$\dot{\mathbf{D}} = f_\phi(\epsilon(\mathbf{t}, \mathbf{D}), \mathbf{D}). \tag{23}$$

The investigation of this *damage evolution equation* gives the key for understanding of failure of brittle materials as the loss of their material stability. The equilibria of (23) and their stability properties give the deformation as the function of the stress and at the same time a fracture or failure criterion of the material.

4.2 Model II. (*Gibbs free energy representation*)

According to the previous representation theorem, the second order polynomial approximation of the Gibbs potential for isotropic materials is

$$\begin{aligned} -\psi(\mathbf{t}, \mathbf{D}) &= (\delta' + k'_\delta \mathbf{D}^2)\mathrm{Tr}\mathbf{t} + (\mu' + \frac{k'_\mu}{2}\mathbf{D}^2)\mathbf{t} : \mathbf{t} + \frac{1}{2}(\lambda' + k'_\lambda \mathbf{D}^2)(\mathrm{Tr}\mathbf{t})^2 + \\ &+ \frac{\alpha}{2}\mathbf{D}^2 + \frac{1}{2}(\beta' + k'_\beta \mathrm{Tr}\mathbf{t})\mathbf{D} \cdot \mathbf{t} \cdot \mathbf{D} + \frac{\gamma'}{2}\mathbf{D} \cdot \mathbf{t} \cdot \mathbf{t} \cdot \mathbf{D}. \end{aligned} \tag{24}$$

Here the notation of the parameters is similar, but constant parameters in one representation result in different, damage and deformation or stress dependent parameters in the other representation according to the definition of the potentials (6). The exceptions are the parameter α, which is the same in both representations and the pure elastic parameters, that are related as we know from linear elasticity ($\mu' = (1+\nu)/2E$ and $\lambda' = \nu/E$, where E is the Young modulus and ν is Poisson's ratio). Therefore the above expression with constant parameters gives a different model from (20). The interpretation of the terms can be given similarly as has been done for Model I.

It is important to put down again the equation of the mechanical equilibrium (the second formula of (8))

$$\begin{aligned} \epsilon \; = \; & (\delta' + k'_\delta \mathbf{D}^2)I + (2\mu' + k'_\mu \mathbf{D}^2)\mathbf{t} + (\lambda' + k'_\lambda \mathbf{D}^2)\mathrm{Tr}\mathbf{t}I + \\ & +(\beta' + k'_\beta \mathrm{Tr}\mathbf{t})\mathbf{D}\circ\mathbf{D} + k'_\beta \mathbf{D}\cdot\mathbf{t}\cdot\mathbf{D}I + \frac{\gamma'}{2}(\mathbf{D}\circ\mathbf{t}\cdot\mathbf{D} + \mathbf{D}\cdot\mathbf{t}\circ\mathbf{D}). \end{aligned} \tag{25}$$

Now the damage strain (the strain at zero stress) is directly calculable:

$$\epsilon_0(\mathbf{D}) := \epsilon(0, \mathbf{D}) = (\delta' + k'_\delta \mathbf{D}^2)I + \beta'\mathbf{D}\circ\mathbf{D}.$$

This particular Gibbs free energy can be considered as a direct generalization of the ideas of Griffith in two different ways, applying the two conditions given in his original paper [35]. First we may accept the interpretation of Rice and Lawn [46, 33] and say that the energy condition can be connected directly to the Gibbs potential. Therefore the thermodynamic force governing the evolution of crack extension is the energy release rate G minus the reversible work W necessary to the crack separation. More properly, in two dimensions, in case of uniaxial tensile loading and a crack perpendicular to the loading axis we can write

$$\psi(t_1, D_1) = W(t_1, D_1) + 2GD_1,$$

where D_1 is the length of the crack, t_1 is the stress, W is the reversible work component and the last term is the specific surface energy.

For perfectly elastic materials we can give the work in a more specific form:

$$W(t_1, D_1) = -\frac{t_1^2}{2E} - \frac{\pi t_1^2 D_1^2}{E}. \tag{26}$$

Here the first term is the pure elastic work, while the second is the work necessary for the reversible crack extension (see e.g. the original work of Griffith [35] or as a thermodynamic treatment the work of Honein at. al. [37]). The expression above is a special form of the Gibbs function (24) for this particular situation, where $\mu' = (1+\nu)/2E$, $k'_\mu = \pi/E$, and the other material parameters are zero.

On the other hand, we can interpret the Griffith theory according to the predictions of the failure threshold of the material. In two dimensions Griffith calculates the following condition for a maximal tensile stress on the crack surface, that can be interpreted as an ultimate failure surface in the stress space for materials containing a lot of randomly oriented microcracks:

$$(t_1 - t_2)^2 + 8K(t_1 + t_2) = 0. \tag{27}$$

Here K is a material parameter depending also on the length of the crack. This equation can be a part of thermodynamic stability as a necessary condition for (9). We can recognize the determinant of the damage related submatrix $\frac{\partial^2 g}{\partial \mathbf{D}^2}(\mathbf{t}, \mathbf{D})$ in the thermodynamic stability condition (9) with special material parameter values in our particular Gibbs free energy function (24).

As in the previous free energy representation, dynamic equations can be given and their properties can be investigated and we can obtain a remarkable correspondence with the observed experimental properties, more details will be given elsewhere [47]. In this paper we restrict ourselves to the treatment of thermodynamic stability thresholds as failure criteria for microcracked materials.

5 Failure and stability

In this section we will investigate the general stability condition derived from the Gibbs free energy (24) with constant parameter values. First of all, let us mention some experimental evidence regarding the strength of rock like materials (concrete, ceramics, etc...) under general loading conditions.

- There is a considerable difference between tensile and pressure strength of rock like materials.
- The damage (failure) surface of these materials has a particular three dimensional shape in the stress space. For example, according to biaxial experiments, contrary to Mohr assumptions, not only the difference of the biggest and lowest principal stresses determine the strength of the rock: the influence of intermediate stresses is not negligible [48].

The three dimensional failure surface produced from the available empirical evidence can be summarized qualitatively on Figure 2. Let us observe the rounded triangle shape on the octahedral plane (cross section perpendicular to the hydrostatic pressure line). The rate dependence of the failure strength observed in experiments makes doubt that this form expresses real material properties [49]. Here we accept the above form as an experimental evidence of the time independent strength surface of materials.

Most of the strength criteria for rocks were suggested for special loading conditions but some of them tries to take into account the above mentioned properties, too. The first and oldest one is the original two dimensional Griffith criterion based on theoretical calculations for single cracks embedded in an elastic domain. Later it was generalized to three dimension by Murell extending some expected properties of the failure surface from two into three dimensions [50, 32]. This criteria suggests a parabolic failure envelope in case of pressure loading and a constant limit stress in case of tensile loading conditions (see also [35, 51]).

Another three dimensional generalization of the criterion of Griffith was used by Theocaris [52, 53] in his Elliptic Paraboloid Failure Criterion. This criterion suggests an elliptic paraboloid open from the hydrostatic axis as initial failure surface in the stress field. It has been proved to be useful to describe the failure of anisotropic materials and results in a better fitting than the criteria of Griffith-Murell. Here the failure loci are given by the next equation at the stress space

$$\mathbf{t} : \mathbf{B} : \mathbf{t} + \mathbf{b} : \mathbf{t} = 1,$$

where **B** and **b** are fourth and second order tensors respectively, they are to be determined experimentally. The parameters should be given in a way that the failure loci form a paraboloid whose axis is the hydrostatic pressure line. Theocaris gives experimental procedures and calculation methods to determine the failure loci from the experiments. Let us remark that the anisotropic property introduced in this criterion is not necessarily a material characteristics, because it can arise from an initially anisotropic damage distribution in case of originally and materially isotropic base continuum, too. On the other hand, the smooth paraboloid seems to be a strong simplification for tensile loadings.

As a third possibility, the best fitting to the measured failure surfaces can be achieved by the criteria of Lade that contains only three material parameters m, η_1 and a,

$$(I_1^3/I_3 - 27)(I_1/p_a)^m = \eta_1, \tag{28}$$

where $I_1 = \mathrm{Tr}(\mathbf{t})$ and $I_3 = \det(\mathbf{t})$ are the first and third invariants of the stress tensor and p_a is the atmospheric pressure. Moreover, the normal stresses contain a translation in the stress space along the hydrostatic axis, the mean stresses t_i in the formula (28) should be replaced with

$$\hat{t}_i = t_i + ap_a \qquad \text{where} \quad i = 1, 2, 3.$$

The corresponding material parameters has been calculated for several rocks from the available (three dimensional) experimental data [48].

All the three criteria are empirical, they were suggested without any serious theoretical justification. In the following we will see that the thermodynamic stability condition of our simple model with one vectorial internal variable can give a comparable fitting, moreover, it has a strong theoretical background as a direct thermodynamic generalization of Griffith criteria in three dimensions. To show this we give here a simple example based on the experimental data of Brown performed on Wombeyan marble with brush plattens [54].

Figure 3 shows the results of biaxial experiments and the corresponding fitted failure surface of Lade and the failure surface proposed by the thermodynamic stability condition. The empty dots denote the experimental results and the thick line is the threshold of the criterion of Lade with the parameter values $m = 1.162$, $\eta_1 = 601500$ and $a = 38.0$. The thermodynamic criterion results in the three finer curves. Their internal hull gives the boundaries of thermodynamic stability. The parameters with the appropriate physical dimensions in SI units are $\delta' = 0$, $k'_\delta = 10.9976 \cdot 10^{-6}$, $\mu' = 23 \cdot 10^{-12}$, $k'_\mu = 3 \cdot 10^{-14}$, $\lambda' = -2.8 \cdot 10^{-12}$, $k'_\lambda = 0$, $\alpha = 100$, $\beta' = 11.2156 \cdot 10^{-6}$, $k'_\beta = 0$, $\gamma' = 3.53 \cdot 10^{-14}$. Only three parameters were used for the fitting, the other non-zero parameters are calculated from the known properties of the material or estimated suitably.

The initial damage vector was chosen as $\mathbf{D} = (0.003, 0.003, 0.003)$, supposing a uniform damage. Here the chosen particular values are not too important, because the failure surface is independent on the damage if it is sufficiently small. It can be seen on the figure that the thermodynamic condition gives a piecewise differentiable failure threshold (like Griffith, but on an other ground).

Let us observe some important qualitative differences between the empirical and the thermodynamic criteria. The thermodynamic failure surface is a cross section of several surfaces, therefore it has some vertices. One of the vertices is on the hydrostatic axis for tensile stresses. It is similar to the predictions of the Griffith-Murrel criteria, where also some cross sectional surface was proposed (a very special one).

Figure 4 shows the whole surface. It can be observed that the surface is closed from the side of large hydrodynamic pressures. Naturally, the parameters, and the whole Gibbs function can be specified to include the requirement of an open failure surface from the hydrostatic line. The published data on this experiment is not sufficient to determine all of the thermodynamic parameters (for the fitting we have chosen a suitable parameter set, considering some physical mechanisms).

However, the concept of failure is not clear from an experimental point of view. The material can be kept together even when its internal structure is completely destroyed. As for example it was pointed out by Orowan [51] in the case of Carrara marble in the classical experiments of Kármán. The marble became powdered, chalk like with large lateral pressures, which indicates a change in the internal structure. In this case the previous assumptions on the Gibbs function aimed to describe a microcracked material become invalid, after the phase breaking another Gibbs function should be introduced to characterize the powdered, frictional state.

6 Discussion and Conclusions

In this paper a theoretical concept of *nonequilibrium phase breaking* is proposed as a tool to extend the frame of the phenomenological thermodynamic modeling. As an application of this idea a particular phenomena, the microcrack induced damage is investigated in detail. Two simple internal variable theories were suggested, using a single vectorial internal variable and based on the most general second order approximation of the Helmholtz and Gibbs free energies, respectively. We have seen that both models can be considered as generalizations of traditional continuum damage mechanical models. Furthermore, the domains of thermodynamic stability and frozen internal variables were suggested as a thermodynamic interpretation of the experimentally measured linear elastic domains in microcracked materials. The boundary of the stable cracking domain, that is the thermodynamic stability was proved to be a generalization of traditional mechanical localization criteria. A comparison with other empirical criteria showed that our suggested theoretical criteria results in a better fitting to the available experimental data in a three dimensional stress space.

The dynamical properties of the model are not investigated in this paper, but it is clear that our simple model can be considered only as a first approximation. The orientation sensitivity of the Kaiser effect, the fact that the microcracking is initiated separately in different orientations is surely not included in our model with a single averaging type internal variable. However, as the present study shows, to propose an irreversible thermodynamic modeling of the evolution of the whole microcrack distribution function seems to be promising.

Let us remark here that several lattice models suggest the impossibility of a 'mean field' description. According to the present investigations, this view cannot be accepted without any reservations, because the investigations use very special loading conditions, the considered molecular interactions are too simple to treat more general cases. Moreover, the applied ideas from nucleation models developed for fluid systems are based on a different kind of localization mechanisms that seems to be present in solid materials. Namely even the simplest Cahn-Hilliard or Ginzburg-Landau like equations are based on weakly nonlocal continuum models and in solid bodies some different localization mechanisms are present and play an important role, too.

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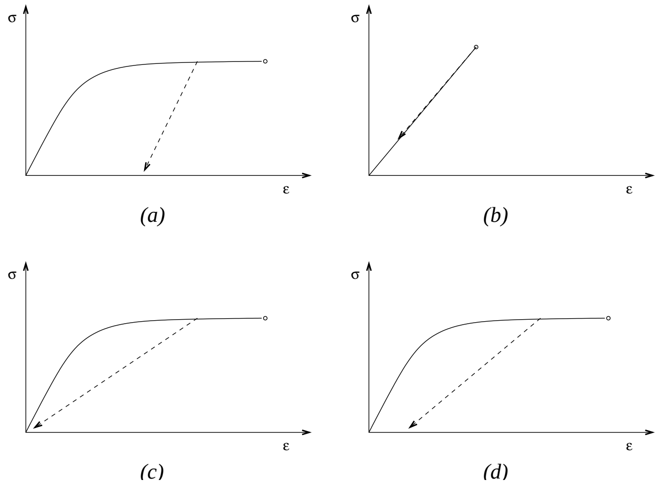
8 Figure captions

- Fig 1 The classification of mechanical materials according to their elastic properties.
- Fig 2 Failure surface from experimental evidence according to Lade [48]
- Fig 3 Biaxial failure envelope, experimental data, the criterion of Lade and the thermodynamic failure surface. The main stresses are given in MPa.
- Fig 4 Thermodynamic failure surface in three dimension



(a) (b)

(c) (d)

Figure 1

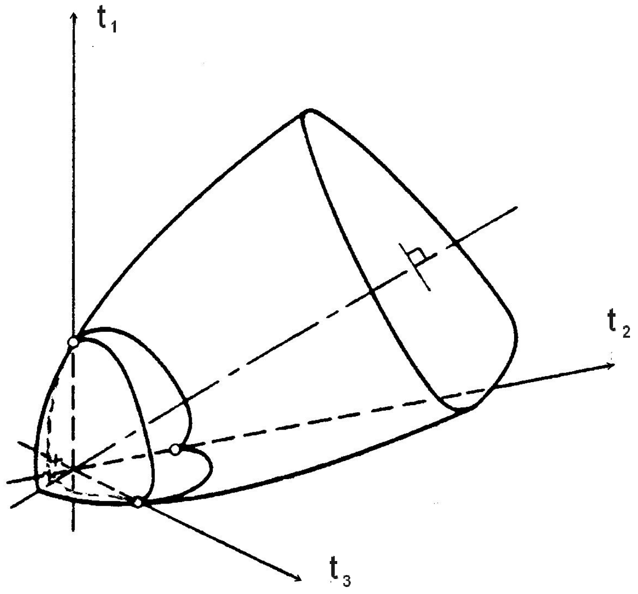


Figure 2

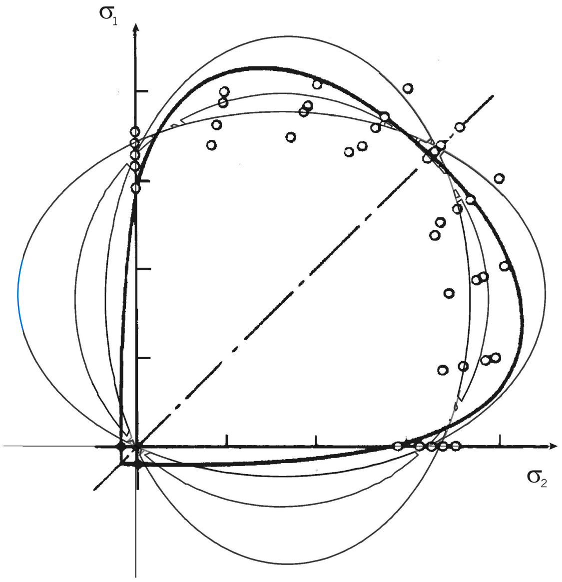


Figure 3

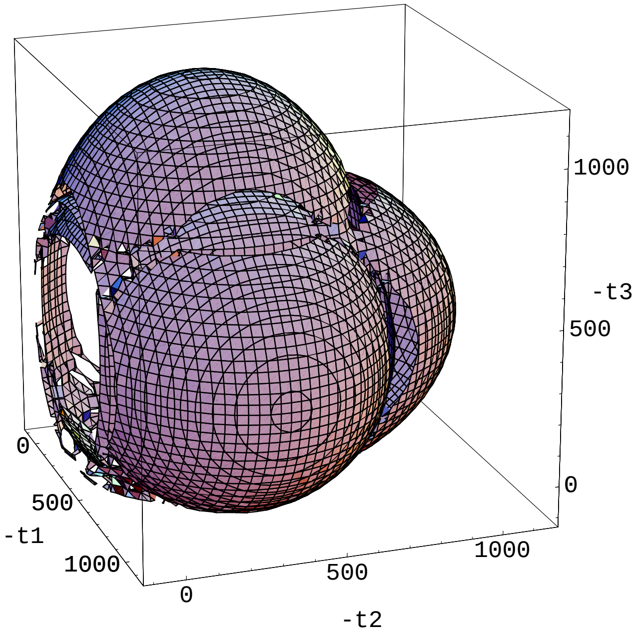


Figure 4