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CONSTITUTIVE MODELING, HETEROGENEITY, THERMODYNAMICS AND MESOMECHANICS OF SOLIDS

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Abstract: *Inelastic macroscopic behavior of technical as well as biological materials is strongly related to their structures. Therefore, constitutive modeling of the respective behavior calls for a description of the influence of structural properties. There are two difficult problems characteristic for this approach:*
(i) It is not sufficient to count only on the average values of stresses and strains in the material constituents. It can be shown that in many important cases the elastic energy of fluctuations of stresses surmounts by order the energy calculated from these average values only.
(ii) In many cases of inelastic deformation it is necessary to take into account the changes in the structure, which is not easy to describe.
In the author's mesomechanical concept, the effect of fluctuations is taken into account by special tensorial internal variables, the changes of state of the material are described by changes of internal mesoscopic stresses and of structural parameters. The last-named changes of structural parameters specify the changes in the structure.

There are many attempts to bypass this problem of structural analysis by using the second law of thermodynamics as a basis for the creation of the respective constitutive equations. Traditionally, phenomenological thermodynamics has been successfully applied in the problems of gases and liquids, but applications to mechanics of solids, specifically in formulations of constitutive equations, meet serious problems. The essential difference between fluids and solids consists in the fact that in solids, a significant amount of mechanical energy can be stored on different structural scales, which makes application of thermodynamics very difficult.

It is shown that the proposed mesomechanical approach leads to results that closely describe the observed behavior of inelastic deformation of many complex heterogeneous materials, that it is simple and general, and the material parameters can relatively easily be determined. It can serve as a basis for a FEM analysis of bodies composed of materials with complicated mechanical and thermomechanical properties.

Key words: *constitutive modeling, mesomechanics, heterogeneity, thermodynamics*

Introduction

Mechanical and thermomechanical macroscopic behavior of technical as well as biological solid materials is strongly related to their structures. Therefore, their constitutive modeling calls for a description of the influence of structural properties. This means taking into account:

(i) Volume fractions of the material constituents.
(ii) Parameters of material properties of the material constituents.
(iii) Internal geometry of the substructures of the material constituents.

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(iv) Description of changes of state of the material including changes in the structure.
(v) Eventuality of several scales of the internal geometry that must be respected.

Taking into account all these factors and finding the way to link them to the macroscopic behavior is of course a very difficult task. To realize it in real materials exactly is impossible. Only approximate models have a chance to succeed. Four important criteria must be taken into account if validating such models:

(a) How close are the results of the model to measured behavior.
(b) How simple is the model.
(c) How general is the model.
(d) How easy is determination of the parameters of the model.

In what follows we are going to comment on several general approaches that try to overcome the difficulties of this complicated problem.

I. Simple models of composites. By this term such models are understood that differentiate the stresses and strains in the material constituents, but under a homogeneous macroscopic loading the respective fields inside these constituents are described as homogeneous. Such models are sometimes used for an approximate description of inelastic processes in composites. In some special cases such a description can give good results, but not generally. The reason is that the elastic energy of fluctuations of the stress field is not of a lower order than the elastic energy of the average values in the material constituents. On the contrary, in many cases the elastic energy of fluctuations (that is neglected in these models) is of a higher order than the energy of the mentioned average values. This has been shown among others by calorimetric measurements, by the X-ray diffraction method, and by the theoretical analysis in the author's publications (Kafka, 1974, 1979, 2001).

II. Thermodynamic theories. Thermodynamic models try to bypass the intricate problem of description of processes in the microstructure by making use of the second law of thermodynamics as a basis for creation of the respective constitutive equations. Traditionally, phenomenological thermodynamics has been successfully applied in problems of gases and liquids. However, application in mechanics of solids, specifically in formulation of constitutive equations, is not so straightforward. The essential difference between fluids and solids consists in the fact that in heterogeneous solids (and nearly all the important materials are heterogeneous on some scale), a significant amount of mechanical energy can be stored on different structural scales. The basis of the thermodynamic approaches – the second law of thermodynamics – can be expressed by the statement that *the internal production of entropy cannot be negative.* In deformation processes, internal production of entropy is expressed by the *irreversible transformation of mechanical energy into heat,* called *dissipation*. Internal production of entropy is usually described by the macroscopically observed plastic work. However, a significant difference exists between the observed plastic work and the real dissipation – due to stored energy that remains in the material. According to calorimetric measurements, the amount of stored energy in polycrystalline metals currently reaches up to 15%, but exceptionally even up to 40% of the macroscopically measurable plastic work (Kafka, 1974, 1979). This means that some not negligible part of the measured plastic work is not dissipated. This fact substantially complicates the use of thermodynamics – not only from the quantitative point of view, but also qualitatively. It is well known that at the end of unloading of specimens of some metallic materials from tensile traction, macroscopic stress can be still positive, but the increase of plastic strain can be negative. If identifying the increase of macroscopically observed plastic work with the entropy production, this would mean that the entropy production would be negative in this phase of unloading. This seeming paradox results from the effect of stored energy (Kafka, 1974, 1979). Hence, it is not possible to identify the entropy production with macroscopically observed plastic work. But without doing it, the use of the second low of thermodynamics is very difficult. The necessary corrections mean questioning at all the significance of thermodynamics in formulation of constitutive equations of solids.

III. Theory of internal variables. In this concept complicated material properties are described by adding a finite number of the so-called 'internal variables' to the common measurable variables. Generality of the resulting relations is restricted by full use of the second law of thermodynamics. A special variant of this approach is the so-called 'endochronic theory', where a special – intrinsic – kind of time is introduced to describe the changes of state of the material in the course of deformation. If the internal variables are not given their specific physical meaning – related to the heterogeneous structure of the material and to the changes of this structure – this approach has the same drawbacks as the above-mentioned 'thermodynamic theories'.

IV. Theory of mixtures. Similarly as in the case of thermodynamic models, theory of mixtures has its origin in applications to fluids and gases. And similarly again, there are problems in applications to solids. Not only the fluctuations of stresses and strains in the heterogeneous system, but also the differentiation of stresses and strains in individual material constituents is here disregarded. Then it is impossible to take into account the important features mentioned above sub (iii) to (v). This model can successfully be used in applications to some special cases of mixtures of a fluid in a solid (as it is the case e.g. in articular cartilage), but surely not as a basis for description of heterogeneous solid-solid systems.

V. Statistical models. These models admit the geometry of composition to be arbitrarily complicated and the microstructure is described by statistical moments. Here, the limiting factors are the input information, which is very demanding to receive, and the very complicated relations that are arrived at in cases of inelasticity. On the top of that it is practically impossible to describe the changes of structure in the course of the deformation process.

In what follows the ways are shown, in which our mesomechanical concept meets the above-specified requirements.

Our Mesomechanical Model

In our mesomechanical concept, macroscopic mechanical properties are identified with the properties of a representative volume element (RVE), loaded at its surface S either by displacements $u_i(S) = \bar{\varepsilon}_{ij} x_j$ or by tractions $t_i(S) = \bar{\sigma}_{ij} n_j$, derived, respectively, from uniform overall strain $\bar{\varepsilon}_{ij}$ or stress $\bar{\sigma}_{ij}$. This identification is justified only in some limits that are discussed in Appendix VIII.1 of our monograph (Kafka, 2001). But outside these limits, measurement of mechanical properties of materials on specimens would be impossible, and consequently experimentally supported constitutive modeling would be impossible either.

(i) Volume fractions of the material constituents are incorporated in the model as fundamental parameters; the sum of the volume fractions is unity. The general form of the model is derived for a finite number of material constituents, concrete applications are based mostly on two-phase schemes; in some cases it was necessary and possible to use three-phase schemes.

(ii) The qualitative form of the constitutive equations of the material constituents is a priori estimated (e.g. elastic, plastic, viscous, fracturing), the respective quantitative parameters must be determined from experiments. The experiments that are necessary for their determination are relatively simple.

(iii) Internal geometry of the substructures of material constituents is described by the so-called 'structural parameters'. Structural parameters corresponding to two substructures labeled by e and n are η^e, η^n. They are deduced (Kafka, 2001) as integral forms in distribution functions describing distribution of microstresses and microstrains under the influence of specific structures. The user of the model does not need to know the distribution functions, he works only with the structural parameters that are relatively easily determinable from experimental stress-strain diagrams. Structural parameters have generally different values for isotropic parts and for deviatoric parts of stresses and strains, but very often in simple variant describing metallic materials only the deviatoric parameters appear. In such a case the distribution of the isotropic parts of stresses and strains is described as homogeneous (volumetric deformations are assumed only elastic and elastic constants are assumed to be homogeneous).

It results from the deduction of the structural parameters that they are non-negative. Finite structural parameters η^e, η^n correspond to continuous substructures, i.e. to substructures that do not form isolated inclusions. If one of the structural parameters – e.g. η^e – is infinite, the substructure of the e-material forms separated inclusions. The higher the value of η^e, the lower is the degree of continuity of the substructure of the e-material. It is a fundamental feature of our model that the degree of continuity and its changes can be described.

From their definition, structural parameters follow as non-negative. But these broad limits can be narrowed. Comparison of our model with exact bounds valid for elastic moduli of heterogeneous bodies led to further limitations (Kafka, Hlaváček, 1995).

Structural parameters describe the shape and continuity of substructures of the material constituents. In the extent of small strains they are considered constant.

(iv) Changes of state of the studied material are described by 'latent variables'.

In the extent of small strains these are internal stresses modeled on the mesoscale by tensors of average stresses in individual material constituents, and by other tensors that describe fluctuations of stresses. It can be shown (Kafka, 2001) that any description based on the average stresses in the material constituents only, cannot be satisfactory.

If describing finite strains, the description of state by only mesomechanical stresses is not sufficient. There start changes in the structure of the material that must be taken into account. In our concept, this is modeled by changes of the structural parameters. Originally, the main field of application of our concept was plastic deformation of ductile polycrystalline materials. In such a case, these changes were described by a progressive loss of continuity of the barriers resisting plastic deformation; a complete loss of continuity of the barriers meant infinite value of the respective structural parameter and rupture.

(v) In its very general form, our model was formulated for a structure composed of a finite number of substructures. However, for concrete applications, to make the model operative and especially to have the possibility of determining the model parameters, it was usually necessary to reduce the number of the substructures to two. But in some cases it turned out that it was not possible to describe the studied material by a two-phase scheme, it was necessary to describe it as a three-phase scheme.

The first material modeled as a three-phase medium was structural concrete (Kafka, 1999). The three substructures were elastic inclusions, elastic-plastic matrix, and substructure of fissures in the matrix.

The other modeled three-phase material was articular cartilage (Kafka, 2002). The three substructures were elastic collagen fibers, elastic matrix, and infiltrated viscous thin constituent of synovial fluid.

Let us further discuss the three aspects mentioned above sub a) to d).

(a) In a number of applications, it was shown that our mesomechanical approach is able to describe the observed macroscopic response to loading very closely. What is considered to be the must significant success, is description of the response to complex loading in ductile polycrystalline metals. The material parameters were determined by a mathematical analysis of a stress-strain diagram of a simple tension test, and with these parameters known it was then possible to describe the response to complex loading. In Figs. 1 to 3 the way of loading, and the respective macroscopic response in a thin-walled aluminum alloy tube is demonstrated.

In the case of structural concrete, the model was more complicated, but it was also possible to find such parameters of the model that give a very close description of the macroscopic response to compressive loading with loops of unloading and reloading – see Fig. 4.

In our monograph (Kafka, 2001) and in a number of papers (Kafka, 1994, 1994a, 1996, 1999, 1999a, 2002; Kafka and Jírová, 1997; Kafka, Jírová and Smetana 1995; Kafka and Karlík, 2001; Kafka and Vokoun, 2000) applications of special variants of our general model to metallic materials, concrete, shape memory materials and biological materials were shown. It was concluded that they give good possibilities of description of their complicated mechanical and thermomechanical properties.

(b) As to the question of simplicity of the model, it is believed that it represents the simplest possible scheme that takes into account different types of substructures and relates them directly to macroscopic properties.

(c) The generality of the model is its strongest point. It covers as special cases the four possible qualitatively different combinations of substructures in a three-dimensional two-phase material: continuous-continuous, discontinuous-continuous, continuous-discontinuous and discontinuous-discontinuous. On the top of that, its very important special feature is the possibility of describing the changes in the microstructure, the changes of the degree of continuity of the substructures. Such changes are characteristic for deformation processes with finite strains.

(d) Determination of material parameters is also relatively simple (Kafka, 2001). It does not require some tedious and expensive microscopic measurements. It starts from relatively simple macroscopic tests followed by a mathematical analysis of the diagrams resulting from them.

Mesomechanical Approach in Modeling Finite Deformations

In the preceding paragraphs, the way of modeling the changes of state of the material were shortly outlined, even for the case of finite strains. However, this does not solve completely the problem of finite strains and finite deformations. In practical applications, it is not only the question of changes of material properties, but also the changes of the form of the studied body that are of essential interest.

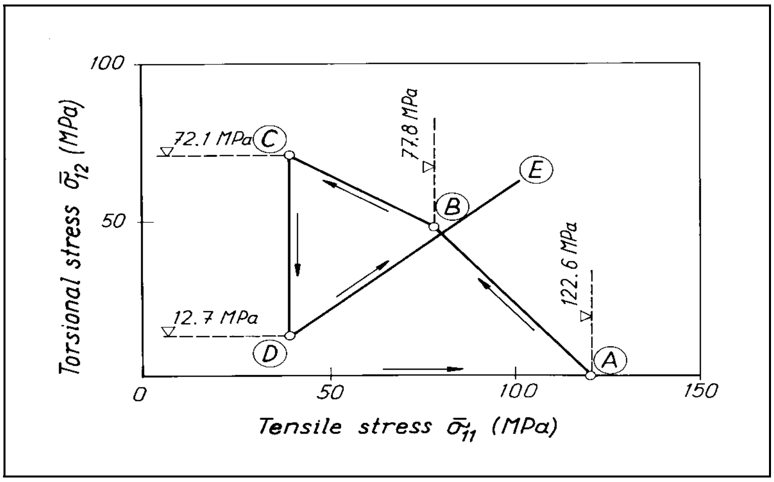

Fig. 1 The complex loading path of the aluminum alloy thin-walled tube

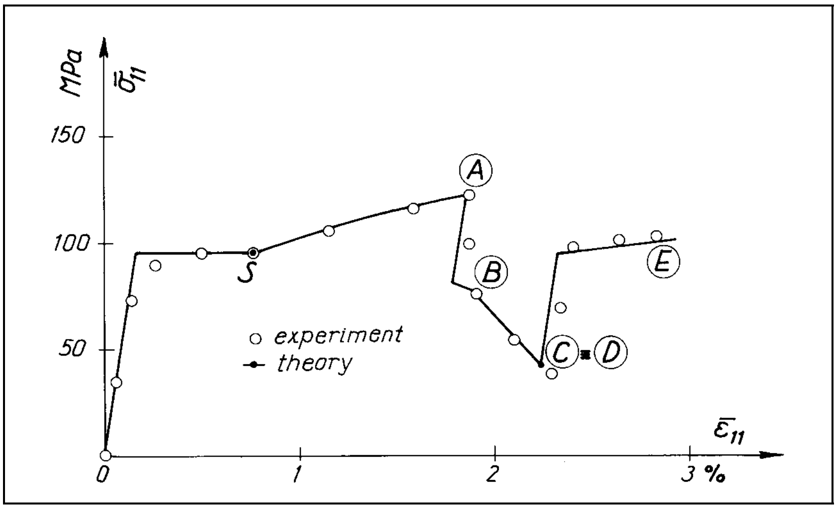

Fig. 2 Theoretical and experimental $\bar{\sigma}_{11} - \bar{\varepsilon}_{11}$ response to the complex loading

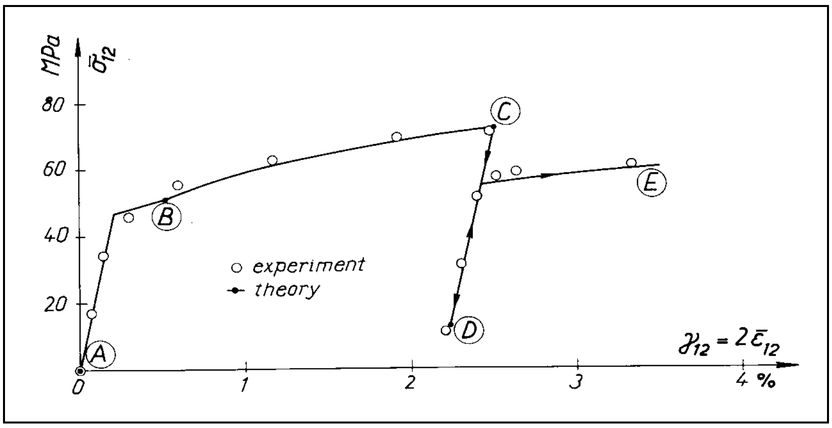

Fig. 3 Theoretical and experimental $\bar{\sigma}_{12} - \bar{\gamma}_{12}$ response to the complex loading

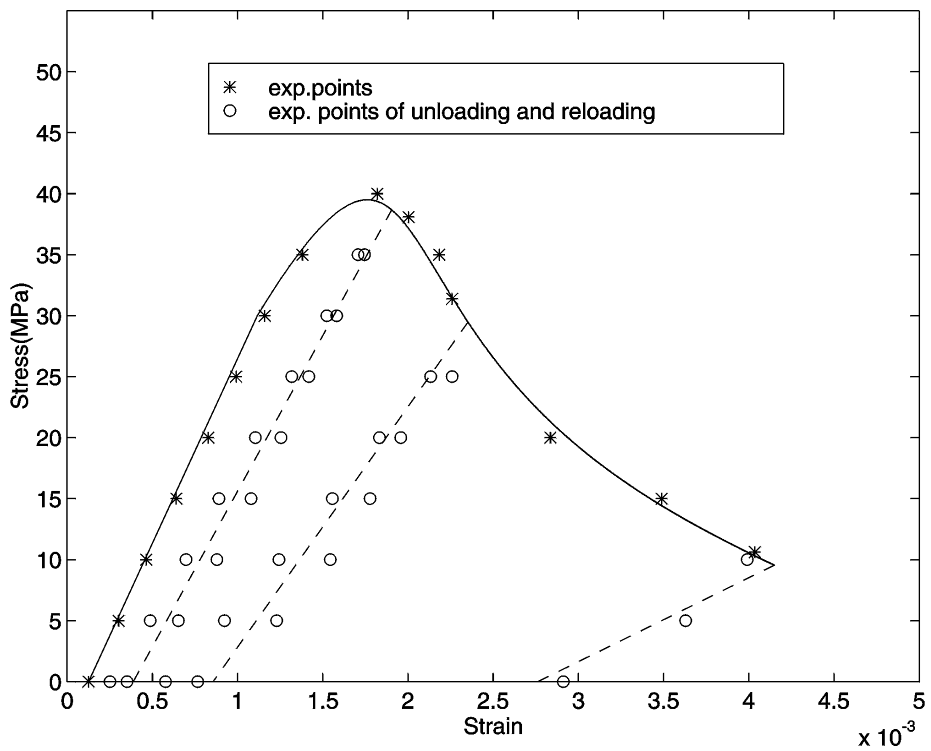

Fig. 4 Model description of the stress-strain diagram of concrete under compression

The simplest case of a tension test of a bar with circular cross-section was analyzed in (Kafka and Karlík, 2001), where the process of cumulative damage and necking in relation to the changes in the structure of material were described. The whole deformation process was divided in very small steps, and after every step not only the respective change of the state of the material, but also the changes of form of the body, of true stress and true strain were taken into account. The uniaxial tension and the circular cross-section made this analysis relatively simple. However, the algorithm used in this analysis can be generalized and used in a FEM procedure.

There are two qualitatively different possible approaches to the problem of describing finite strains and finite deformations in bodies:

- The first one – let us call it the 'integral' approach – relates the current material properties and form of the body to the original 'virgin' state and form, and tries to describe the whole 'deformation path' and development of material properties by some functions or functionals.
- The other one – let us call it the 'differential' approach – concentrates only on one differential step in a small element of the body. In this case it is necessary to know the form of the element, the 'state' of the material in the element, and true stress and true strain in the element. The deformation process is then numerically summed up of differential small deformations, the deformed body is composed of deformed finite elements.

The crucial point in the second 'differential' approach is the description of the state of the material. And this is the important advantage of our mesomechanical model that it offers tensorial three-dimensional description of the state of the material and of the changes of this state in relation to true strain and true stress and their variations. Hence, it offers the way to modeling deformations processes in bodies with complex inelastic and thermoelastic properties.

Conclusion

The mesomechanical model – in confrontation with other approaches – is shown to have a number of merits. These are especially its generality, simplicity and lucidity. Whereas in phenomenological 'black-box' theories the changes of the material properties are usually described by artificially introduced 'back-stresses' or scalar latent variables without specifications of their physical meaning, in the mesomechanical concept tensorial latent variables are clearly specified as internal mesoscopic stresses.

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