D. R. Axelrad · W. Muschik (Eds.)

Recent Developments in Micromechanics

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Preface

This volume contains the lectures presented at the mini-symposium on "Micromechanics" held in conjunction with the CSME Mechanical Engineering Forum 1990 between the 3rd and 8th June, 1990 at the University of Toronto, Canada. The expressed purpose of this symposium was to discuss some recent developments in the Micromechanics of Materials and how advances in this field now relate to the solution of practical engineering problems. Due to the time limit set for this section of the Engineering Forum as well as the restriction on the number of papers to be presented, it was not possible to cover a much wider range of topics. However, an attempt was made to include the most important advances associated with the progress made in micromechanics in its application to material science and engineering over the past decade. Thus, the topics are concerned with:

- the fundamental aspects of the thermodynamics of structured solids (part I),
- the micromechanical behaviour of alloys (part II),
- the modelling of the material behaviour on the basis of continuum theory (part III), and finally
- the important new approach to the characterization of various materials and their responses to external agencies by the use of probabilistic micromechanics (part IV).

We would like to take this opportunity to thank the Chairman of the Organizing Committee, Prof. F.P.J. Rimrott, and the President of the CSME, Prof. T.S. Sankar, for their permission to prepare this publication coincident with the Proceedings of the CSME Engineering Forum 1990. We would also like to express our thanks to the members of the Local Organizing Committee for the support given by them in arranging the various seminars, and the staff of Springer Verlag, in particular Mr. A. von Hagen, for the efficient production of this volume.

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October, 1990

D.R. Axelrad and W. Muschik

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Part I
Thermodynamics of Materials

Non-Equilibrium Thermal/Mechanical Behaviour

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Summary

A solid undergoes nonequilibrium changes when disturbed, a phenomenon that occurs at both the microscopic and macroscopic scale level. These changes depend on the rate at which the process takes place and cannot be described in terms of physical parameters representing the system as a whole. Their description involves synchronizing the thermal fluctuation with mechanical motion of the material at each location and time.

The concept of an isoenergy density space is introduced such that the energy state in a volume element can be characterized by the time history of only one stress and one strain component regardless of whether the element is in a uniaxial or multiaxial state of stress. A unique correspondence between the uniaxial and multiaxial stress state can thus be established without loss in generality. Unlike the classical approaches in continuum mechanics, the response of an isoenergy density element requires the simultaneous specification of element size, time and temperature. Mutual interaction of size/time/temperature cannot be ignored for nonequilibrium states because temperature averaged over a macroelement within a given time interval can differ qualitatively and quantitatively from that over a microelement and different time interval. The same applies to mechanical motion.

As an example, data for the nonequilibrium thermal/mechanical response of an aluminum cylindrical bar specimen stretched at a displacement rate of 1.27×10^{-4} cm/sec will be presented. A two-phase medium is considered such that the conditions at the solid/air interface are allowed to change with time rather than specified or ignored as in the classical treatment of equilibrium processes. Thermal/mechanical disturbances are found to prevail in the surrounding of the specimen; they diminished at distances more than one-half the specimen length. The response is transitory in character for the entire load history and depends on the initial thermal environment next to the specimen as well as the rate of the applied external disturbance.

Introduction

A physical system is said to be in a state of nonequilibrium when its constituents change continuously with time in a nonhomogeneous fashion. That is, the thermal/mechanical properties cannot be described by parameters representing the system as a whole. Traditional approaches have relied on *statistics* and *kinetics* for developing molecular models where conditions of irreversibility at both the microscopic and macroscopic scale level are imposed. While numerical data have been obtained for coefficients in the transport equations, they cannot be readily used in engineering application.

Theories of nonequilibrium *thermodynamics* [1-3] are equally unsatisfying for they do not consider the mutual interaction of temperature change with the motion of mass elements. Thermal and mechanical effects are left unsynchronized. Inhomogeneity being characteristic of the nonequilibrium process cannot be adequately described by applying the same equation of state or constitutive relation to all mass elements in a system. Moreover, the linear relation assumed for the entropy *exchanged* between the system and surrounding and that *generated* in the system is also disturbing because it excludes the possibility of interaction between the heat exchanged and generated. These limitations can be overcome only if thermal change and mechanical motion are considered intrinsically as one of the same operation.

As a fundamental departure from the classical field theories, the isoenergy density theory [4,5] takes into account the change of element size that no longer shrinks to zero. The elements can expand and/or contract depending on the local rotation and deformation without restrictions in magnitude and finiteness. They are known as the isoenergy density elements because their orientation and size are determined at each location and time increment according to the load history from the condition that the same energy is transmitted across all the mutually orthogonal surfaces. Unique correspondence of energy state between uniaxial and multiaxial stress/strain state is thus made possible without loss in generality. A brief summary of the isoenergy density theory will be given for the sake of continuity.

Isoenergy Density Theory

The change of volume with surface denoted by $\Delta V/\Delta A$ or $\mathcal{V}$ is assumed to vanish in the limit when the element size is shrunk indefinitely. This assumption will no longer be made in the isoenergy density theory [4,5]. For an orthogonal coordinate system in three dimensions, the three components $\mathcal{V}_j$ ($j = 1,2,3$) establish the relations the components $\mathcal{S}_j$ ($j = 1,2,3$) of the surface energy density vector and the volume energy density $\mathcal{W}$ as

$$\mathcal{S}_j = \mathcal{V}_j \cdot \mathcal{W}, \quad j = 1,2,3 \tag{1}$$

A system of rectangular Cartesian coordinates ξ_i ($i = 1,2,3$) is used to locate the surfaces of energy transmission.

Isoenergy Element. An isoenergy surface possesses the property that the transmission of energy on such a surface is directional independent. If ξ_i ($i = 1,2,3$) are the current state coordinates, then the condition

$$S_1 = S_2 = S_3 \to S \tag{2}$$

determines the position of the element that the same S prevails on all orthogonal surfaces. On the isoenergy surface, the scalar W has a unique form

$$W = \iint \lambda V \mathrm{dede} \tag{3}$$

where λ defines a particular isoenergy density state and the limits of integration; it can depend on e. Equations (1) and (2) imply that

$$V_1 = V_2 = V_3 \to V \tag{4}$$

The finiteness of V makes the theory nonlocal. General expressions for the rate change of volume with surface V can be found in [5] where deformation, rotation and change in element size are combined into one operation. In equation (3), e stands for any one of the nine displacement gradients

$$e_{ij} = \frac{\partial u_i}{\partial \xi_j}, \quad i,j = 1,2,3 \tag{5}$$

with u_i being the displacement components.

Thermal/Mechanical Interaction. Mass elements deform and change temperature simultaneously. Interdependence of these two effects cannot be assumed as a priori but must be determined [4,5]:

$$\frac{\Delta\Theta}{\Theta} = -\lambda V \frac{\Delta e}{\Delta \mathcal{D}/\Delta e} \tag{6}$$

in which Θ represents the nonequilibrium temperature in contrast to T in classical thermodynamics that applies only to equilibrium states. The dissipation energy density $\mathcal{D}$ is determined on the isoenergy density plane; it is a positive definite quantity and its differential change can be written as

$$d\mathcal{D} = dW - dA, \quad \mathcal{D} \geq 0; \ \frac{d\mathcal{D}}{dt} \geq 0 \tag{7}$$

with A being the available energy. Since the dissipated and available energy are defined to be mutually exclusive, the linear relation of equation (7) remains valid in general and is equivalent to the conservation of energy. Because Θ can be determined from V, e and $\mathcal{D}$ without heat, the isoenergy density formulation represents a fundamental departure from thermodynamics. Irreversibility is reflected through the H-function:

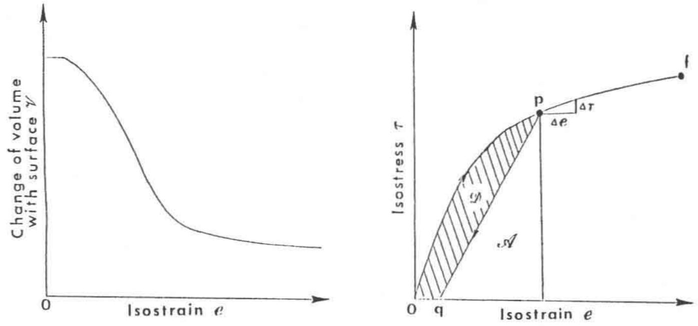
$$dH = - \frac{d\mathcal{D}}{\Theta} \tag{8}$$

The negative sign indicates work is done on the system. The change of H can be positive, zero or negative. It is not related to the Boltzmann H-theorem in statistical dynamics for dilute gases.

Isostress and Isostrain. Since an isoenergy density state is completely defined by (V,e) as W in equation (3), there is no need for the stress quantity. A theory can be formulated using the concept of force alone would be sufficient. For the sake of familiarity, however, the isostress τ referred to isoenergy density plane will be defined:

$$\tau = \int \lambda V de \tag{9}$$

such that λ can depend on e as mentioned earlier. A one-to-one correspondence between (V,e) and (τ,e) is invoked by equation (9) and is illustrated in Figures 1(a) and 1(b). A unique feature of the isoenergy density theory can be stated as follows:



(a) γ versus e (b) τ versus e

Fig. 1. Equivalence of slope on isostress and isostrain curve to change of volume with surface

The state of an isoenergy element defined by (V,e) or (τ,e) is determined for each load step and time increment without a preknowledge of the so-referred to "constitutive relations" in classical field theory.

Only the relation between τ and e for the reference state of a material is required. Once the loading steps are specified, adjustment on (τ,e) is made for each load step at every location in the system. A new curve opf as shown in Figure 1(b) is found for each element.

Recovery State. Each material has the capability to recover even though the process may not be completely reversible. There is a definite path pq for each isolated element in a system. Such a path should be distinguished from that of unloading for a uniaxial specimen because the tractions on an isolated element will not vanish even when the external disturbances or loads are completely removed from the body. The local recovery path is assumed to follow that of the reference state for determining the path pq and hence the dissipation energy density $\mathcal{D}$ or the available energy density A. In view of equation (9), equation (6) also takes the form

$$\frac{\Delta\Theta}{\Theta} = -\frac{\Delta\tau\Delta e}{\Delta\mathcal{D}} \tag{10}$$

This illustrates how Θ is found for each increment change of $\Delta\tau$ and Δe, Figure 1(b).

Governing Equations. As in the classical field theories, the governing equations can be derived by application of the conservation of linear and angular momentum and conservation of energy. Nonequilibrium, nonlocal, irreversible, and large/finite deformation effects are also included in addition to having finite element size. This necessitates the distinction between the Cauchy stress $\underset{\sim}{\sigma}$ and isostress $\underset{\sim}{\tau}$ which are related as

$$\tau_{ij} = \sigma_{ij} + \rho(\ddot{u}_i - h_i)\mathcal{V}_j \tag{11}$$

The quantities $\rho\ddot{u}_i$ and ρh_i represent the inertia and body force, respectively, while ρ is the mass density and dot stands for differentiation with time. The isostress tensor $\underset{\sim}{\tau}$ is not symmetric on account of the non-local character of the deformation. The conservation of energy applied to a system with volume Λ enclosed by surface Σ yields

$$\int_\Lambda \rho h_i \dot{u}_i dV + \int_\Lambda \overset{n}{T}_i \dot{u}_i dA = \int_\Lambda \rho\ddot{u}_i \dot{u}_i dV + \frac{d}{dt}\int_\Lambda \mathcal{W} dV \tag{12}$$

With n_i being the components of the outward unit normal vector, the tractions are given by

$$\overset{n}{T}_i = \tau_{ji} n_j, \quad \tau_{ij} \neq \tau_{ji} \tag{13}$$

Derivation of equation (12) also reveals that

$$\mathcal{W} = \tau_{ij}\dot{e}_{ij} \tag{14}$$

Make note that $\mathcal{W}$ is not an elastic potential. It applies to an irreversible and dissipative process as implied by equations (7) and (8). The equations of equilibrium are

$$\frac{\partial \tau_{ji}}{\partial \xi_j} + \rho h_i = \rho \ddot{u}_i \tag{15}$$

Existence and Boundness. The existence of the isoenergy density function $\mathcal{W}$ has been proved in [5]. Only the theorem will be given as follows:

There exists an isoenergy density function $\mathcal{W}$ that can be obtained by integrating λV twice with respect to any one of the nine displacement gradients $\partial u_i/\partial \xi_j$ (i,j = 1,2,3) where V is the change of volume with surface for a given λ.

Mathematical equivalence of the foregoing statement is that

$$\mathcal{W} = \int \tau_{11}de_{11} = \int \tau_{12}de_{12} = \dots = \int \tau_{23}de_{23} \rightarrow \int \tau de \tag{16}$$

This means that any one of nine pairs (τ_{11},e_{11}), $(\tau_{12},e_{12}),\dots,(\tau_{23},e_{23})$ or (τ,e) can be used to yield the same $\mathcal{W}$. Hence, the uniaxial isostress τ versus isostrain e plot provides a general representation of the energy state even though the other stress components τ_{ij} are also acting on the isoenergy element.

Because nonequilibrium implies nonuniqueness, uniqueness proof can be provided only for equilibrium states [5]:

Isoenergy equilibrium states (V,e) or (τ,e) are unique for positive definite isoenergy density function $\mathcal{W}$, and the satisfaction of equilibrium and continuity.

The nonequilibrium fluctuation of isoenergy states can only be bounded by their neighboring equilibrium states. Boundness and limit have been rigorously established and can be summarized [5]:

Fluctuations of nonequilibrium/irreversible isoenergy states are bounded by equilibrium/irreversible isoenergy states and they tend to definite limits depending on the initial step.

What can be deceiving is that the outward appearance of some of the governing equations in the isoenergy density theory may be similar to those in ordinary mechanics; the underlying principles and assumptions are completely different. The departure begins from the start in equation (1) where the exchange of S and V does not take place in ordinary mechanics.

Cooling/Heating of Uniaxial Specimen

The uniaxial tensile specimen has been used extensively for obtaining basic mechanical properties such that the data can be used in the design of more complex systems. A basic assumption is that the stress and/or strain state within certain gage length can be regarded as constant or in equilibrium. Such an idealization would encounter considerable difficulties if a wide range of loading rates, specimen sizes and environmental conditions are considered. For instance, specimens tested under varying temperature conditions are more sensitive to change in strain rate, geometry and/or size. Classical thermo-mechanical theories based on equilibrium considerations [6] cannot be applied in principle to explain the nonequilibrium cooling/heating phenomenon. Agreements between theory and experiment are contrived. This can be evidenced from the wrong deduction [7] made by the same thermo-viscoplasticity theory [6] that torsional loading produced no reversal of heat flow. Experiments [8] at Lehigh University showed that the effect of cooling/heating is just as pronounced in torsion as in extension. Synchronization of thermal change with mechanical deformation remains to be accomplished. The specification of temperature or its gradient on the solid surface is another idealized assumption that cannot be justified on physical grounds because it ignores the possible interaction between the solid and its surrounding. This can, in turn, affect the bulk behavior of the uniaxial specimen and interpretation of the data.

Thermally and Mechanically Induced Deformation. Without making a priori assumption on the temperatures or temperature gradients distribution that prevail on the uniaxial tensile specimen, the far field temperature is maintained uniform at a prescribed value to be denoted by Θ_0. The temperature changes and displacements of the mass elements in both the solid and its surrounding will be found. A schematic of the two-phase system is given in Figure 2 in which the circular cylinder occupies the region R_2 enclosed by Σ_2 is engulfed by the air in region R_1 with boundary Σ_1 on which Θ_0 is maintained constant. The solid specimen is stretched at a displacement rate of $\dot{u} = 1.27 \times 10^{-6}$ m/sec.

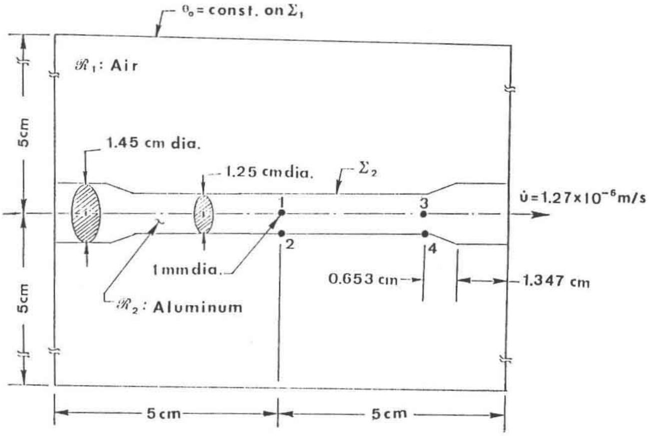


Fig. 2. Schematic of aluminum tensile specimen in air environment with temperature Θ_0

The influence of four different far field temperatures Θ_0 = 25°, 75°, 125° and 175°C will be investigated [9]. A sufficiently small load increment load is first taken so that the properties of the solid and air can be assumed to be known and thus preassigned. All subsequent responses will be determined individually for each solid and fluid element and time step. Table 1 gives the initial values of $d\tau/de$ for the 6061 aluminum and air at different values of Θ_0. Following the procedure discussed in [5], results will be obtained for t = 120,240,...,720 sec.

Table 1 Reference properties of 6061 aluminum and air

Temperature Θ_0 (°C)	Initial Slope $d\tau/de \times 10^5$ (Pa)	
	6061 $A\ell$	Air
25°	8.167×10^5	2.0
75°	7.500	2.5
125°	6.500	3.0
175°	5.000	3.5

Local and Global Behavior. The nonequilibrium stress and strain behavior can be seen from the difference between the local and global response as illustrated in Figures 3 and 4 for Θ_0 = 25°C. Referring to the four typical locations 1, 2, 3 and 4 in Figure 2, it is seen that the isostress and isostrain curves differed in the nonlinear range. Along the centroidal axis of cylinder where dilatational effect is more pronounced, the elements would experience a higher strain rate. This is indicated by curves 1 and 3 in