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SOME THOUGHTS ON MATERIAL STABILITY.(U)
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by

R. S. Rivlin

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Some Thoughts on Material Stability

by

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Abstract

The paper is concerned with some underlying physical considerations which bear on the development of restrictions on the strain-energy function for an elastic material which may undergo finite deformations. Some comments are also made on the possible use of the strain-energy function at deformations for which a necessary condition for material stability is violated.

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1. Introduction

The main difficulty which arises in discussing material stability is any clear concept in physical terms of what the term implies. We have only the vague notion that some restrictions should be placed on constitutive equations, other than those which result from invariance under superposed rigid motions and material symmetry, to ensure that the material modelled is well-behaved physically. However, the precise sense in which the material is to be well-behaved is not entirely clear.

Nevertheless, we can recognize certain physical behavior which is clearly unacceptable, i.e. certain situations can be recognized as evidencing instability. This fact enables us to discuss in a meaningful way necessary conditions for material stability even though it may be fruitless to attempt to obtain sufficient conditions.

In classical elasticity theory certain restrictions can be placed on the elastic moduli, the violation of which implies material instability. For an isotropic material, these are the conditions that the shear and compression moduli both be positive. They result from the fundamental consideration that if either of the moduli is negative, the material will undergo a deformation from its assumed initial homogeneous state even though no forces are applied to it. However, even in this case, it is by no means evident that the assumption of positive shear and compression moduli are sufficient to ensure stability. That this is the case is evident from the discussion in §§5 and 6 of

the role of thermal and other fluctuations in effecting instability.

The search for necessary conditions for material stability of isotropic elastic materials subjected to finite deformations has been greatly influenced by the corresponding problem in classical elasticity theory. However, physical points of departure, which in the classical infinitesimal theory lead to the same conditions on the elastic moduli, when transposed into the context of finite elasticity theory may lead to quite different restrictions on the strain-energy function. We shall not, in this paper, discuss the various rather complicated restrictions on the strain-energy function for isotropic elastic materials which have been obtained. Rather, we will concentrate on some rather general considerations of a physical character which provide the basis for such relations. We shall also make some comments on the possible use of a strain-energy function at deformations for which one or other of the necessary conditions for material stability is violated. It is emphasized that these comments are advanced tentatively and are intended only to draw attention to certain questions which arise when a strain-energy function is used at such deformations.

2. Infinitesimal deformations

If an isotropic elastic material is subjected to infinitesimal deformations, the strain-energy W per unit volume is given by

$$W = \frac{1}{2}\lambda(\mathrm{tr}\ \underset{\sim}{e})^2 + \mu\,\mathrm{tr}\ \underset{\sim}{e}^2 , \tag{2.1}$$

where $\underset{\sim}{e}$ is the infinitesimal strain matrix and λ and μ are the Lamé constants for the material. $\underset{\sim}{e}$ is defined in terms of the displacement vector $\underset{\sim}{u}$ by

$$\underset{\sim}{e} = \frac{1}{2}\{\underset{\sim}{\nabla}\underset{\sim}{u} + (\underset{\sim}{\nabla}\underset{\sim}{u})^{\dagger}\} , \tag{2.2}$$

where the dagger denotes the transpose.

A possible definition of material stability, in this case, is that W is positive definite. That this is a necessary condition is evident from the fact that if W is negative for some $\underset{\sim}{e}$, the material will be unstable in its undeformed state. The condition that W be positive definite is easily seen to be equivalent to the conditions

$$\mu > 0 , \quad 2\mu + 3\lambda > 0 . \tag{2.3}$$

In physical terms, the conditions (2.3) state that the shear and compression moduli must be positive. Together they imply that

$$\lambda + \mu > 0 , \tag{2.4}$$

i.e. the equibiaxial plane strain modulus is positive. The conditions (2.3) and (2.4) together imply that Young's modulus E is positive, i.e.

$$E = \frac{\mu(2\mu+3\lambda)}{\lambda+\mu} > 0 \ . \tag{2.5}$$

However, (2.4) and (2.5) do not imply (2.3) and hence do not provide sufficient conditions for W to be positive definite. Nor can one of the conditions (2.4) and (2.5) be taken with one of the conditions (2.3) to imply that W is positive definite.

A necessary condition for material stability which is sometimes considered is the Hadamard condition that the speeds of all plane waves, propagated in a body of the material filling three-dimensional space, be positive. The necessary and sufficient conditions for this to be the case are

$$\mu > 0 \ , \quad \lambda + 2\mu > 0 \ . \tag{2.6}$$

These conditions are equivalent to the condition that the acoustic tensor be strongly elliptic. The second of the conditions (2.6) also has the statical interpretation that the tensile modulus, when the dimensions normal to the direction of stretch are fixed, be positive.

While the conditions (2.3) imply the conditions (2.6), the converse is not true. Accordingly, the Hadamard conditions are weaker than the condition that W be positive definite.

If the deformations are infinitesimal, we do not distinguish

between the Cauchy stress $\underset{\sim}{\sigma}$ and the Piola-Kirchhoff stress $\underset{\sim}{\Pi}$. They are given by

$$\underset{\sim}{\sigma} = \underset{\sim}{\Pi} = \partial W/\partial \underset{\sim}{e} \ . \tag{2.7}$$

It can easily be seen that the condition that W be positive definite is equivalent to the condition that it be a convex function of $\underset{\sim}{e}$. The convexity of W can be expressed algebraically as

$$W(\underset{\sim}{e}_2) - W(\underset{\sim}{e}_1) > \mathrm{tr}\{(\underset{\sim}{e}_2-\underset{\sim}{e}_1)\underset{\sim}{\Pi}_1\} \ , \tag{2.8}$$

where $\underset{\sim}{e}_1$ and $\underset{\sim}{e}_2$ are two strains and $\underset{\sim}{\Pi}_1$ and $\underset{\sim}{\Pi}_2$ are the corresponding stresses. The condition (2.8) is in turn equivalent to the condition

$$\mathrm{tr}\{(\underset{\sim}{\Pi}_2-\underset{\sim}{\Pi}_1)(\underset{\sim}{e}_2-\underset{\sim}{e}_1)\} > 0 \ . \tag{2.9}$$

If the elastic material is anisotropic, it can still be shown quite easily that positive definiteness of W is equivalent to convexity expressed by either of the conditions (2.8) or (2.9).

3. An attempted generalization

It is evident that if we remove the condition that the deformations be infinitesimal, positive semi-definiteness of W, regarded as a function of the deformation gradients, remains a necessary condition for material stability. It is then tempting to try to find equivalent convexity conditions with which to replace the convexity conditions (2.8) and (2.9) which are valid for the case of infinitesimal deformations. Such a generalization was attempted by Coleman and Noll [1] in 1959.

They considered a deformation in which a particle initially in vector position $\underset{\sim}{X}$ moves to $\underset{\sim}{x}$. Let $X_A (A=1,2,3)$ and $x_i (i=1,2,3)$ be the components of $\underset{\sim}{X}$ and $\underset{\sim}{x}$ respectively in a rectangular cartesian coordinate system. Then the deformation gradient matrix $\underset{\sim}{g}$ is defined by

$$\underset{\sim}{g} = ||g_{iA}|| = ||\partial x_i/\partial X_A|| \ . \tag{3.1}$$

The strain-energy W, per unit initial volume, is then a scalar function of $\underset{\sim}{g}$. Coleman and Noll [1] suggested that the convexity condition (2.8) be replaced by the condition

$$W(\underset{\sim}{g}_2) - W(\underset{\sim}{g}_1) > \mathrm{tr}\{(\underset{\sim}{g}_2-\underset{\sim}{g}_1)\underset{\sim}{\Pi}_1\} \ , \tag{3.2}$$

where $\underset{\sim}{g}_1$ and $\underset{\sim}{g}_2$ are the deformation gradient matrices corresponding to any two deformations related by

$$\underset{\sim}{g}_2 = \underset{\sim}{s}\underset{\sim}{g}_1 \ , \tag{3.3}$$

where $\underset{\sim}{s}$ is a symmetric matrix, and $\underset{\sim}{\Pi}_1$ and $\underset{\sim}{\Pi}_2$ are the corresponding Piola-Kirchhoff stress matrices*. The relation (3.3) implies that the deformation corresponding to $\underset{\sim}{g}_2$ may be obtained from that corresponding to $\underset{\sim}{g}_1$ by superposing on the latter a pure homogeneous deformation. The condition (3.2), with (3.3), has been called by Truesdell and Toupin [2] the C-N condition, and they showed that it is equivalent to the condition

$$\mathrm{tr}\{(\underset{\sim}{g}_2-\underset{\sim}{g}_1)(\underset{\sim}{\Pi}_2-\underset{\sim}{\Pi}_1)\} > 0 \ , \tag{3.4}$$

which they called the GCN condition.

That the C-N and GCN conditions are not necessary conditions for material stability is evident from a much earlier result obtained by Rivlin [3] in 1948. He considered the pure homogeneous deformation of a unit cube of incompressible neo-Hookean material by specified forces acting normally to its faces and uniformly distributed over them. If the strain-energy W is given in terms of the principal extension ratios $\lambda_1,\lambda_2,\lambda_3$ by

$$W = \frac{1}{2}\, C(\lambda_1^2+\lambda_2^2+\lambda_3^2-3) \ , \tag{3.5}$$

where C is a positive constant, then the applied forces f_1,f_2,f_3 are given by

$$f_i = C\lambda_i - p/\lambda_i \quad (i=1,2,3) \ , \tag{3.6}$$

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* $\underset{\sim}{\Pi}_1 = ||\Pi_{Ai}^{(1)}|| \ , \ \underset{\sim}{\Pi}_2 = ||\Pi_{Ai}^{(2)}|| \ .$

where p is a hydrostatic pressure which is arbitrary if the λ's are specified. Since the material is incompressible, the λ's must satisfy the relation

$$\lambda_1\lambda_2\lambda_3 = 1 \ . \tag{3.7}$$

If the f's are specified, then equations (3.6) and (3.7) provide four simultaneous equations for the determination of the λ's and p. These do not necessarily have a unique solution and consequently if the applied forces are specified the resultant equilibrium states of pure homogeneous deformation may not be uniquely determined. Certain of these equilibrium states may be unstable and which of the stable states is attained will, in general, depend on the manner in which the applied forces are increased from zero to their final values.

For example [4], if the f's are all equal and tensile, i.e. $f_1 = f_2 = f_3 = f$, say, with $f > 0$, there are seven possible pure homogeneous equilibrium states:

(i) $\lambda_1 = \lambda_2 = \lambda_3 = 1$

(ii) $\lambda_1 = \lambda_2 \ , \ \lambda_3 < \frac{1}{3} f/C$

(iii) $\lambda_1 = \lambda_2 \ , \ f/C > \lambda_3 > \frac{1}{3} f/C$

and states obtained from (ii) and (iii) by cyclic permutation of the subscripts on the λ's.

The state (ii) and the two further states obtained from it are stable, while the state (iii) and the two further states obtained from it are unstable. The undeformed state (i) is stable

or unstable accordingly as $f/C < 2$ or > 2 .

It was shown by Truesdell and Toupin [2] that if the C-N or GCN conditions are satisfied, the relation between the forces and principal extension ratios for pure homogeneous deformation of a cube of the material are uniquely invertible. Accordingly, these conditions are not satisfied by an incompressible neo-Hookean material to which three equal tensile forces are applied, even if these are small. Since materials exist for which the neo-Hookean strain-energy function is fairly accurately valid and which show no evidence of material instability, we conclude that the C-N and GCN conditions are not necessary conditions for material stability. A heroic attempt was made by Truesdell and Noll [5] to salvage these conditions as necessary for material stability. They asserted that the C-N and GCN conditions should be applied only to compressible materials. However, they failed to explain how the unique invertibility of the force-principal extension ratio relations for a slightly compressible material can, in the limiting case when the material is incompressible, yield multiple widely-separated equilibrium states of pure homogeneous deformation for specified forces.

The condition that the strain-energy function, regarded as a function of $\underset{\sim}{g}$, be globally convex may be expressed as

$$W(\underset{\sim}{g}_2) - W(\underset{\sim}{g}_1) > \mathrm{tr}\{(\underset{\sim}{g}_2-\underset{\sim}{g}_1)\Pi_1\} , \tag{3.8}$$

where $\underset{\sim}{g}_2$ and $\underset{\sim}{g}_1$ are the deformation gradient matrices corresponding to any two states of deformation, not necessarily connected

by the relation (3.3).

Since the C-N and GCN conditions are less severe restrictions on the strain-energy function than global convexity, the latter is not a necessary condition for material stability.

Local convexity at a point may be expressed by the relation

$$\delta^2 W > 0 \ , \tag{3.9}$$

where $\delta^2 W$ denotes the second variation of W at that point. This may, in turn, be written as

$$\frac{\partial^2 W}{\partial x_{i,A} \partial x_{j,B}} \ \delta x_{i,A} \delta x_{j,B} > 0 \ , \tag{3.10}$$

for all arbitrary variations $\delta x_{i,A}$ of the deformation gradients. The relation (3.10) may be rewritten as

$$\delta \Pi_{Ai} \delta x_{i,A} > 0 \ , \tag{3.11}$$

where $\delta \Pi_{Ai}$ is the variation in the Piola-Kirchhoff stress corresponding to the variation $\delta x_{i,A}$ in the deformation gradients. In matrix notation (3.11) becomes

$$\mathrm{tr}(\delta \underset{\sim}{\Pi} \delta \underset{\sim}{g}) > 0 \ . \tag{3.12}$$

Although we do not know whether the local convexity condition (3.11) is a necessary condition for material stability,

it certainly becomes such if certain restrictions are placed on the variations $\delta x_{i,A}$, $\delta \Pi_{Ai}$ and on the underlying Piola-Kirchhoff stress Π_{Ai} . Illustrations of such cases are given in the next section. In each of them the total work in the incremental deformation is done by only one of the components of $\underset{\sim}{\Pi}$.

We denote this component of $\underset{\sim}{\Pi}$ by f and the corresponding deformation gradient by ε . Then, the condition (3.11) becomes

$$\delta f \delta \varepsilon > 0 \; ; \tag{3.13}$$

i.e. the f-ε relation must have positive slope. This is evidently a necessary condition for material stability. The implications of its violation will be discussed in §5. The condition (3.13) is, of course, equivalent to the condition that the incremental modulus μ defined by

$$\mu = \partial f / \partial \varepsilon \; , \tag{3.14}$$

be positive.

4. Some restricted convexity conditions

In this section we describe certain situations in which the local convexity condition (3.11) reduces to the form (3.13) and accordingly provides a necessary condition for material stability. In each of these situations a rectangular block of elastic material, not necessarily isotropic, with its edges parallel to the axes of a rectangular cartesian coordinate system $\bar{x}$, is assumed to undergo a pure homogeneous deformation with principal extension ratios $\lambda_1, \lambda_2, \lambda_3$ and principal directions parallel to the axes of the system $\bar{x}$.

We consider a rectangular block of the material to be cut from the parent block, with edges parallel to the axes of a rectangular cartesian coordinate system x which may or may not coincide with the system $\bar{x}$. This is held in its deformed state by appropriate forces. We now superpose on the deformation existing in this block an infinitesimal static deformation. For our purposes this is most conveniently described in the coordinate system x.

Case 1. The system x has arbitrary orientation with respect to the system $\bar{x}$ and the infinitesimal superposed deformation consists of a simple shear with the x_1-direction as the direction of shear and the x_1x_2-plane as the plane of shear. The incremental shear modulus must then be positive for material stability.

Case 2. The system x has an arbitrary orientation with respect to the system $\bar{x}$ and the infinitesimal superposed deformation is a pure homogeneous deformation with one principal direction parallel to the x_1, say, axis, while the dimensions of the block parallel to the x_2 and x_3 axes are held fixed. We shall call this constrained simple extension. The incremental modulus in

the 1-direction must then be positive for material stability. It is evident, however, that this condition becomes meaningless when the material is incompressible.

Case 3. The system x has one axis, say x_2, parallel to one of the axes, say $\bar{x}_2$, of the system $\bar{x}$, but is otherwise of arbitrary orientation. In the underlying pure homogeneous deformation, the faces of the block normal to $\bar{x}_2$ are force-free and remain so in the infinitesimal superposed deformation which is pure homogeneous and has principal directions parallel to the axes of the system x and zero extension in the x_3, say, direction. The incremental tensile modulus must then be positive for material stability.

Case 4. The system x has all of its axes parallel to those of the system $\bar{x}$, while both the initial finite and superposed infinitesimal deformations are simple extensions parallel to one of the axes, say x_1. The incremental tensile modulus must then be positive for material stability.

The restrictions which these conditions impose on the strain-energy function for an isotropic elastic material have been and remain the subject of extensive investigation. The results which have already been obtained are often complicated and in some cases surprisingly difficult to achieve. We shall not pursue this rather intricate matter here.

5. Instability for one-dimensional deformations

In this section we shall discuss simplistically the extension e by a tensile force f of a thin uniform weightless rod of elastic material with initial length L. We assume that f increases monotonically with e for values of e below some value e_m at which f has the maximum value f_m. For higher values of e, f is assumed to decrease monotonically with increase in e. The f-e relation is shown schematically in Fig.1(a). The portion of the f-e curve on which the modulus $\mu = df/de$ is positive is denoted I. That on which it is negative is denoted II.

The energy W stored elastically in the rod is given by

$$W = \int_0^e f(e)de \ , \tag{5.1}$$

and

$$f(e) = \frac{dW(e)}{de} \ . \tag{5.2}$$

The dependence of W on e is shown schematically in Fig.1(b) and we note that W increases monotonically with e, but has a point of inflexion when $e = e_m$.

Suppose the rod is held, with its ends fixed, in the homogeneous state of deformation corresponding to the point P_1 on the portion II of the f-e curve. Then, $f,e = f_1, e_1$, say. Now, suppose the applied force is reduced to f_2. If the extension increases to e_2, as we might expect from Fig.1(a), so that the point P_2 is reached, the work done is $(e_2-e_1)f_2$, while the increase in strain-energy is $\int_{e_1}^{e_2} f(e)de$. Since

$$(e_2-e_1)f_2 < \int_{e_1}^{e_2} f(e)de \ , \tag{5.3}$$

the deformation cannot take place. The question arises - what will, in fact, occur? We shall defer discussion of this until later in this section.

Again, suppose that the rod is held, with its ends fixed, in the homogeneous state of deformation corresponding to the point P_1 in Fig.1(a) and now the constraint on one end of the rod is removed so that a dead-load f_1 acts on the rod. If the extension of the rod increases to e_2, the work done by the dead-load is $(e_2-e_1)f_1$ and the strain-energy increases to $\int_{e_1}^{e_2} f(e)de$. Since

$$(e_2-e_1)f_1 > \int_{e_1}^{e_2} f(e)de \ , \tag{5.4}$$

the deformation can take place and when the extension e_2 is attained the load will have a kinetic energy of amount

$$(e_2-e_1)f_1 - \int_{e_1}^{e_2} f(e)de \ . \tag{5.5}$$

If a homogeneous equilibrium state can be attained by the rod, the f-e curve must reverse slope, either as shown in Fig.2(a) or in Fig.2(b). We denote by III the rising portion of the curve beyond the extension at which the minimum value of f occurs.

We now return to the situation in which the rod is held with its ends fixed a distance $L + e$ apart. We shall, however, not assume that the rod is homogeneously deformed. Let ℓ be the

distance, in the undeformed state, of a generic particle of the rod from one end. Let $\varepsilon(\ell)$ be the strain at this particle in the deformed state and let $w(\varepsilon)$ be the strain-energy per unit initial length. Then, the total strain-energy W in the rod is given by

$$W = \int_0^L w(\varepsilon)d\ell \ . \tag{5.6}$$

The kinematic constraint on the rod is expressed by

$$\int_0^L \varepsilon(\ell)d\ell = e \ . \tag{5.7}$$

For equilibrium, the first variation δW of W must be zero, for all variations $\delta\varepsilon(\ell)$ of $\varepsilon(\ell)$ which satisfy the constrain condition (5.7) and hence the condition

$$\int_0^L \delta\varepsilon(\ell)d\ell = 0 \ . \tag{5.8}$$

With (5.6), we obtain

$$\delta W = \int_0^L \frac{dw(\varepsilon)}{d\varepsilon}\,\delta\varepsilon(\ell)d\ell = 0 \ . \tag{5.9}$$

Taking account of the constraint (5.8) by introducing the (constant) Lagrange multiplier $-f$, we obtain from (5.9)

$$f = dw(\varepsilon)/d\varepsilon \ . \tag{5.10}$$

f is the tension in the rod. Thus, the equilibrium state of the

rod is characterized by the condition that the tension is constant throughout the rod.

From Fig.2 we see that the following possibilities exist:

(i) The rod is homogeneously deformed.

(ii) Part of the rod is in one state and the remainder in another state; these are states corresponding to the constant value of f which lie on two of the three segments I, II, III.

(iii) Parts of the rod are in each of three states. These are the three states corresponding to the constant value of f which lie on the segments I, II, III of the f-e curve.

We now consider the stability of these possible equilibrium states.

An equilibrium state is unstable if the second variation $\delta^2 W$ of W is negative for some kinematically possible variation $\delta\varepsilon(\ell)$ of $\varepsilon(\ell)$. From (5.6) and (5.10), we have

$$\delta^2 W = \frac{1}{2}\int_0^L \frac{d^2 w(\varepsilon)}{d\varepsilon^2}(\delta\varepsilon)^2 d\ell = \frac{1}{2}\int_0^L \frac{df(\varepsilon)}{d\varepsilon}(\delta\varepsilon)^2 d\ell \ . \qquad (5.11)$$

In case (i) when the rod is homogeneously deformed, $df(\varepsilon)/d\varepsilon$ and hence $\delta^2 w$ is negative if the extension of the rod corresponds to a point on the segment II of the f-e curve. The corresponding equilibrium state is, accordingly, unstable. We observe that this instability certainly obtains as soon as the extension e_m is passed and we shall see later that it may arise earlier.

We now pass to case (ii). We consider an equilibrium state in which a part ℓ_1 of the rod, of total initial length L_1, is subjected to a uniform strain ε_1, while the strain in the remainder ℓ_2, of total initial length L_2, is also uniform but of magnitude ε_2. Let $w(\varepsilon)$ be the strain-energy per unit initial length when the strain is ε. Then, the total strain-energy W in the rod is given by

$$W = L_1 w(\varepsilon_1) + L_2 w(\varepsilon_2) \ . \tag{5.12}$$

We have also

$$L = L_1 + L_2 \ , \quad e = L_1\varepsilon_1 + L_2\varepsilon_2 \ . \tag{5.13}$$

We obtain from (5.12)

$$\delta W = w(\varepsilon_1)\delta L_1 + w(\varepsilon_2)\delta L_2 + L_1 \frac{dw(\varepsilon_1)}{d\varepsilon_1}\,\delta\varepsilon_1 + L_2 \frac{dw(\varepsilon_2)}{d\varepsilon_2}\,\delta\varepsilon_2 \ . \tag{5.14}$$

From (5.13) we obtain the kinematic constraints on δL_1, δL_2, $\delta\varepsilon_1$, $\delta\varepsilon_2$:

$$\delta L_1 + \delta L_2 = 0 \ , \ L_1\delta\varepsilon_1 + L_2\delta\varepsilon_2 + \varepsilon_1\delta L_1 + \varepsilon_2\delta L_2 = 0 \ . \tag{5.15}$$

The equilibrium condition $\delta W = 0$ for all kinematically possible variations $\delta L_1,\ldots,\delta\varepsilon_2$ yields

$$\frac{dw(\varepsilon_1)}{d\varepsilon_1} = \frac{dw(\varepsilon_2)}{d\varepsilon_2} = f \ , \quad \text{say} \ , \tag{5.16}$$

and

$$w(\varepsilon_2) - w(\varepsilon_1) = f(\varepsilon_2 - \varepsilon_1) \ . \tag{5.17}$$

The relation (5.16) expresses the fact that at equilibrium the tensions in the parts L_1 and L_2 of the rod are equal. The relation (5.17) is the well-known Maxwell relation. If ε_1 and ε_2 correspond to points B,C lying on the segments I and II of the f-ε curve, as shown in Fig.3, the relation (5.17) cannot be satisfied for any value of f, since $w(\varepsilon_2) - w(\varepsilon_1)$ is the area of the vertically hatched region in Fig.3, while $f(\varepsilon_2 - \varepsilon_1)$ is the necessarily smaller area of rectangle ABCD.

Similarly, if ε_1 and ε_2 correspond to points C,F lying on the segments II and III of the f-ε curve, the relation (5.17) cannot be satisfied for any value of f, since $w(\varepsilon_2) - w(\varepsilon_1)$ is the area of the horizontally hatched region in Fig.3 and $f(\varepsilon_2 - \varepsilon_1)$ is the necessarily greater area of the rectangle DCFE.

However, if ε_1 and ε_2 correspond to the points B,F lying on the segments I and III of the f-ε curve, as shown in Fig.4, the relation (5.17) can be satisfied by choosing f so that the striated areas above and below the line f = constant are equal. This line f = constant is sometimes called the Maxwell line. We emphasize that the critical value of f and hence those of ε_1 and ε_2 are independent of the detailed shape of segment II of the f-ε curve and depend only on the area under it. It can be shown that the equilibrium state determined in the above manner is stable.

Since the value of f corresponding to the Maxwell line determines ε_1 and ε_2, if c is specified L_1 and L_2 can

be determined from equations (5.13).

This analysis is, of course, dependent on the assumption that an element of the rod can pass freely between the states of strain ε_1 and ε_2. For this to be the case, thermal or other fluctuations must be present of sufficient magnitude to allow the tension in the element to reach the value of f corresponding to the maximum of the f-ε curve, at any rate instantaneously.

It will be recognized that the model outlined above is in accord with that presented in texts on thermodynamics for isothermal reversible first-order phase transitions.

Now suppose that fluctuations of sufficient magnitude, for the processes outlined above to take place, are not present. Then the overall extension of the rod, at which transitions in a part of it to strain values corresponding to points on segment III take place, is greater than that determined by the Maxwell line. In the limiting case when there are no fluctuations, it will reach the value $L\varepsilon_m$. Then, as the overall extension $L\varepsilon_m$ is exceeded the transition takes place dynamically and the calculation of the manner in which it occurs would be rather complicated and, indeed, there is some doubt that it could be carried out purely on the basis of the f-ε curve of the type considered so far. The reason for this doubt will appear more clearly in the next section, in which is discussed a specific physical situation in which force-induced transitions from one twinning mode to another take place in quartz.

If the force f is applied as a dead load, as soon as it reaches the value f_m, a transition will take place in the whole

rod to the point on the segment III of the f-e curve corresponding to this value of f. The kinetic energy of the load will then be

$$f_m L(\varepsilon_2-\varepsilon_1) - [w(\varepsilon_2)-w(\varepsilon_1)] .$$

The rod will accordingly oscillate about this state and if the material has any internal friction will eventually reach equilibrium at the point on III corresponding to the load f_m.

We will now show that the situation (iii) in which parts ℓ_1, ℓ_2, ℓ_3 of the rod are in three different states corresponding to points on segments I, II, III respectively of the f-ε curve does not represent a possible equilibrium condition for the rod.

Let L_1, L_2, L_3 be the total initial lengths of ℓ_1, ℓ_2, ℓ_3 respectively and let ε_1, ε_2, ε_3 be the strains in them in the deformed state in which the total extension of the rod is e. Then,

$$L_1 + L_2 + L_3 = L , \quad L_1\varepsilon_1 + L_2\varepsilon_2 + L_3\varepsilon_3 = e . \qquad (5.18)$$

The total strain-energy W is given by

$$W = L_1 w(\varepsilon_1) + L_2 w(\varepsilon_2) + L_3 w(\varepsilon_3) . \qquad (5.19)$$

The equilibrium condition $\delta W = 0$ for all kinematically possible variations $\delta L_1,\ldots,\delta\varepsilon_3$ yields

$$\frac{dw(\varepsilon_1)}{d\varepsilon_1} = \frac{dw(\varepsilon_2)}{d\varepsilon_2} = \frac{dw(\varepsilon_3)}{d\varepsilon_3} = f \ , \quad \text{say} \ ,$$

and (5.20)

$$w(\varepsilon_2) - w(\varepsilon_1) = f(\varepsilon_2 - \varepsilon_1) \ , \quad w(\varepsilon_3) - w(\varepsilon_2) = f(\varepsilon_3 - \varepsilon_2) \ .$$

By reasoning similar to that used in discussing case (ii) it is evident that the last two relations in (5.20) cannot be satisfied.

So far we have considered extension of the rod and the concomitant transition of the whole or parts of it from states on segment I to states on segment III of the f-ε curve. If such transitions have taken place and we now decrease the extension quasistatically, then provided that the fluctuations are large enough for the tension in the rod to decrease below the value of f corresponding to the minimum on the f-ε curve, the whole process will be reversed and transitions will take place from the state on segment III to the state on segment I determined by the Maxwell line. If the fluctuations are not large enough for this to occur, extension of the rod will have to be further reduced before a transition can take place.

Finally, we note that whether or not the rod can rest in two different states when the tension in it is zero will depend on whether segment III of the f-ε curve does or does not intersect the abscissa of the f-ε curve (see Fig.2). If such an intersection exists, the rod will have an equilibrium state with zero tension provided that the fluctuations are not too large.

6. Force-induced change of twinning mode in quartz

Quartz is crystalline silica, SiO_2 . It can exist in two crystalline forms, the so-called α-form, which is normally stable at ordinary temperatures and the β-form which is the stable form above 573°C.

α-quartz, the form with which we shall be concerned here, belongs to the trigonal-trapezohedral symmetry class (32). It has a single axis of three-fold rotational symmetry, usually called the optic axis, and, in the plane perpendicular to this, three axes of two-fold rotational symmetry, often called electric axes, as shown schematically in Fig.5. The crystal has no plane or center of symmetry.

Structurally, a crystal of α-quartz consists of tetrahedra at the corners of which the oxygen atoms are located. A silicon atom is located at the center of each tetrahedron, and each oxygen atom is chemically bonded to two silicon atoms. If we start at, say, a silicon atom we can trace out a helix, with its axis parallel to the optic axis, on which lie a succession of silicon-oxygen-silicon-oxygen atoms. This helix may form a left-handed or a right-handed screw. As a result of this screw-like structure, if a beam of plane-polarized light is transmitted parallel to the optic axis, its plane of polarization is rotated and we distinguish between left-handed and right-handed quartz accordingly as the plane of polarization is rotated in the sense of a left-handed or right-handed screw. A single crystal of α-quartz may consist in part of left-handed and in part of right-handed quartz and is then said to be optically twinned. We shall not be concerned with this type of twinning here.

There is, however, another type of twinning which occurs in α-quartz. This is called Dauphiné, or electrical twinning, and occurs in the following way. We have a crystal for which the optic axis is, say, the outward drawn normal to the paper in Fig.5. The crystal consists entirely of left-handed quartz or entirely of right-handed quartz. However, in part of the crystal, the electric axes are directed as shown in Fig.5(a) while in the remainder they are rotated from these directions through 180° about the optic axis, i.e. as shown in Fig.5(b).

If a plate of an untwinned crystal is cut with its major surfaces normal to one of the electric axes and compressed by forces acting on these surfaces, an electrical potential difference is developed across the plate, i.e. the crystal is peizoelectric. For an electrically twinned plate the magnitude of the potential difference is reduced as a result of the fact that the potential differences produced in the differently oriented parts of the plate are of opposite sign.

It can be seen by examining a model of the structure of quartz that a crystal oriented as shown in Fig.5(b) can be converted into one oriented as shown in Fig.5(a) by relatively small displacements of the individual oxygen atoms relative to the silicon atoms.

It is found experimentally that an electrically twinned crystal of, say, left-handed α-quartz can in certain circumstances be converted to an untwinned crystal of the same hand by the application of appropriate forces. This process is greatly facilitated by raising the temperature of the crystal unti it approaches or exceeds the α-β transition temperature and then

cooling it before removal of the forces.

An effective method [6] of promoting this transition is to cut from an untwinned crystal of α-quartz a rectangular plate with its length perpendicular to the optic axis. The plate is subjected to torsion by means of couples about the length direction. If the couple is large enough the plate will transform into a crystal of the opposite twin (equivalent to a rotation of the structure through 180° about the optic axis) except in narrow layers at the two free edges. The magnitude of this force depends on the angle θ between the normal to the plate and the optic axis and on the angle ϕ between the projection of this normal on the plane perpendicular to the optic axis and the positive direction of a two-fold symmetry axis.

W.A. Wooster and N. Wooster [6] measured the torsional couple necessary to produce a change from one twinning mode to the other as a function of θ and ϕ. The results they obtained are illustrated in the three-dimensional polar diagram of Fig.6, in which the optic axis is vertical and the polar distance is proportional to the inverse of the torque necessary to produce the transformation. The upper lobes, labelled with a + sign, relate to transformation in one direction and the lower ones, labelled with a - sign, to transformation in the opposite direction. The maxima on the upper lobes correspond to $(\theta,\phi) = (45^{\circ},30^{\circ})$, $(45^{\circ},150^{\circ})$, $(45^{\circ},270^{\circ})$ and those on the lower lobes to $(\theta,\phi) = (135^{\circ},30^{\circ})$, $(135^{\circ},150^{\circ})$, $(135^{\circ},270^{\circ})$. In addition to these lobes, Wooster and Wooster found six further similar lobes which are not shown in Fig.6. Three of these, with maxima at $(\theta,\phi) = (135^{\circ},90^{\circ})$, $(135^{\circ},210^{\circ})$, $(135^{\circ},330^{\circ})$, relate to transformation in

the same direction as the upper lobes shown. The remaining three, with maxima at $(\theta,\phi) = (45^\circ,90^\circ)$, $(45^\circ,210^\circ)$, $(45^\circ,330^\circ)$, relate to transformation in the opposite direction.

In [7] and [8], W.A. Wooster and Thomas proposed a theory to explain these experimental results, based on the assumption that whether or not a transformation will take place, when the plate is subjected to dead-loading by a torque, is determined by the difference in the total energies of the system with the plate in the transformed and untransformed states. We denote these energies by E_T and E_U respectively. Then, if $E_U > E_T$, the transformation will take place; otherwise it will not. It is further assumed that if $E_U > E_T$ the torque required to produce the transformation is a monotonically decreasing function of $E_U - E_T$. This energy difference can be easily calculated from the known elastic constants of α-quartz.

When the plate is subjected to a torque, the stress in the plate is predominantly a shearing stress which increases linearly with distance from the axis of torsion. We denote the appropriate shear compliances for the material of the plate in its transformed and untransformed states by κ_U and κ_T respectively.

Then, it can easily be seen that $E_U - E_T$ is given by an expression of the form

$$E_U - E_T = C(\kappa_T - \kappa_U)M^2 , \tag{6.1}$$

where M is the applied torque and C is a positive constant which depends on the dimensions of the plate. The compliances κ_T and κ_U can both be calculated from the known compliance

matrix for α-quartz, $\kappa_T - \kappa_U$ being given by an expression of the form

$$\kappa_T - \kappa_U = \kappa \sin 2\theta \sin 3\phi \ , \tag{6.2}$$

where κ is a constant. It is easily seen that, with (6.2), equation (6.1) yields a three-dimensional polar diagram, in which the radial distance from the pole is proportional to $E_U - E_T$, of the same general form as Fig.6.

The experimental fact, already noted, that the transformation from one twinning mode to another does not take place near the free edges of the plate is easily explained by the theory. To do so we note that when a thin plate is subjected to a torsion, the shearing stress at the free edges must be zero.

The theory outlined above can evidently be generalized, at any rate in principle, to other types of deformation and bodies of other geometries. However, the predictions are not always in accord with the experimental observations. This may be due to the fact that as soon as a change of twinning mode has been initiated at one point of the body, we are faced with a boundary-value problem involving an inhomogeneous body. The stress distribution associated with the prescribed loading may then be very different from that which was assumed to exist either initially or in the final state when complete transformation has taken place. Furthermore, the theory considers only a quasistatic change from one twinning mode to another and does not take account of the dynamics of this transformation.

It can easily be seen that a theory of the dynamics of the

transformation from one twinning mode to the other cannot be based on an elastic strain-energy function which depemds on the macroscopic deformation gradients alone. Presumably when a load is applied to the crystal, the relative positions of the oxygen and silicon atoms change, for sufficiently small loads, in a reversible fashion, and, at any instant, depend on the current value of the deformation gradient matrix. Accordingly, for sufficiently small loads the stress can be determined from a strain-energy function which depends only on the current value of the deformation gradient matrix. However, when some critical value of the load is reached, this configuration becomes unstable and the atoms snap into a new relative configuration. During this snap-through the relative positions of the oxygen and silicon atoms will not depend in a unique fashion on the macroscopically measured value of the macroscopic deformation gradient matrix and accordingly the stress cannot be derived from a strain-energy function which depends only on the deformation gradient matrix. If the positions of the oxygen atoms relative to the silicon atoms are described by appropriate internal variable fields, then it may be possible, in principle, to derive the stress from a strain-energy function which depends on these fields as well as on the deformation gradient matrix. However, for this to be the case it would be necessary that in the snap-through of the atoms from positions appropriate to one twinning mode to positions appropriate to the other twinning mode, no significant amount of energy is irreversibly communicated to internal degrees of freedom of the atoms.

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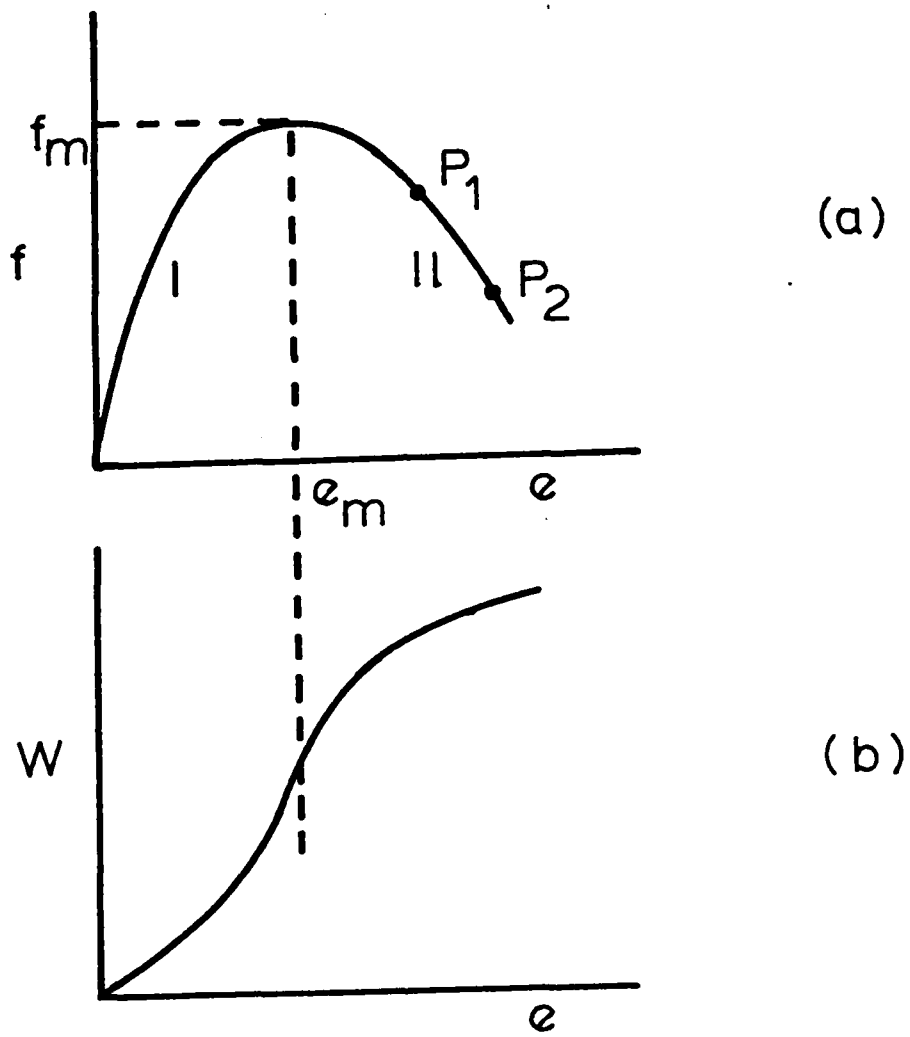


FIG.1

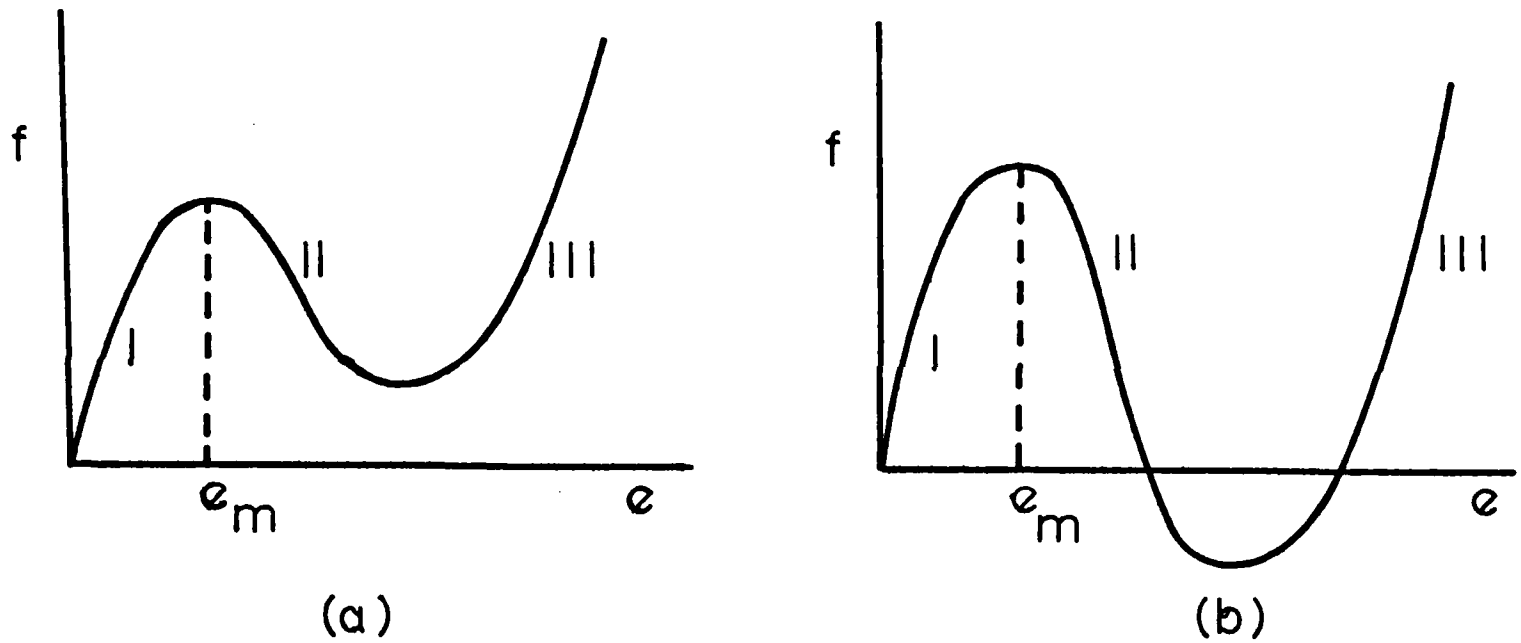
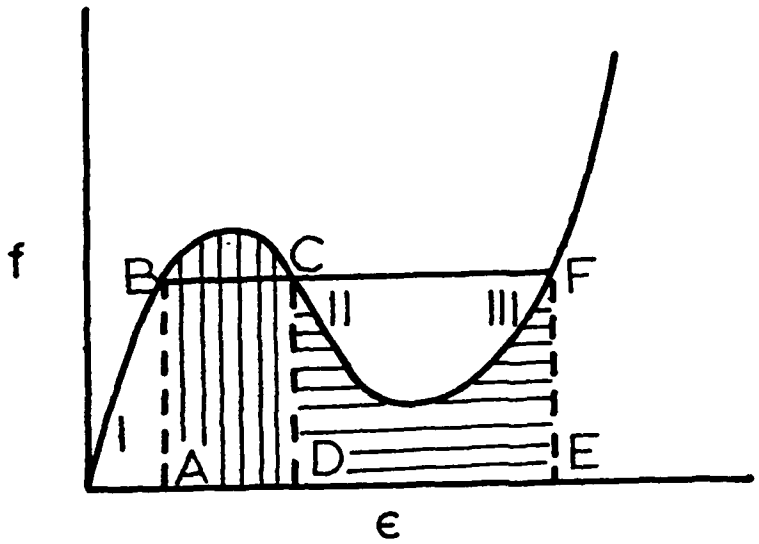


FIG. 2



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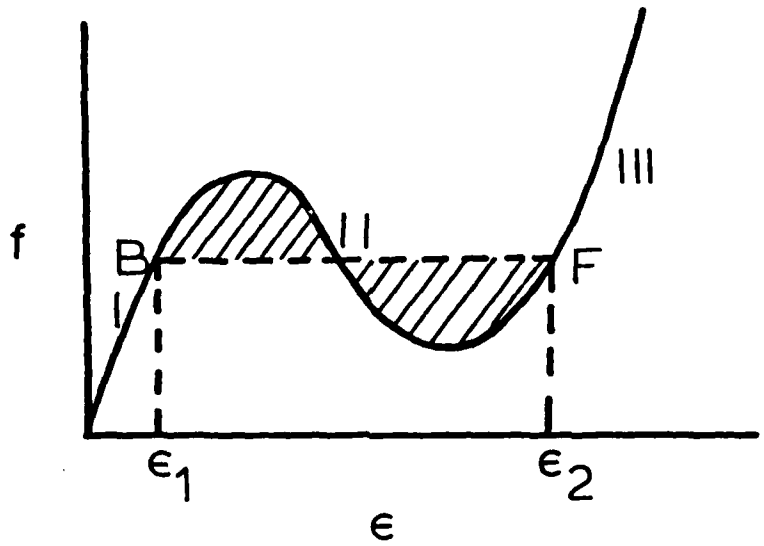

FIG. 4

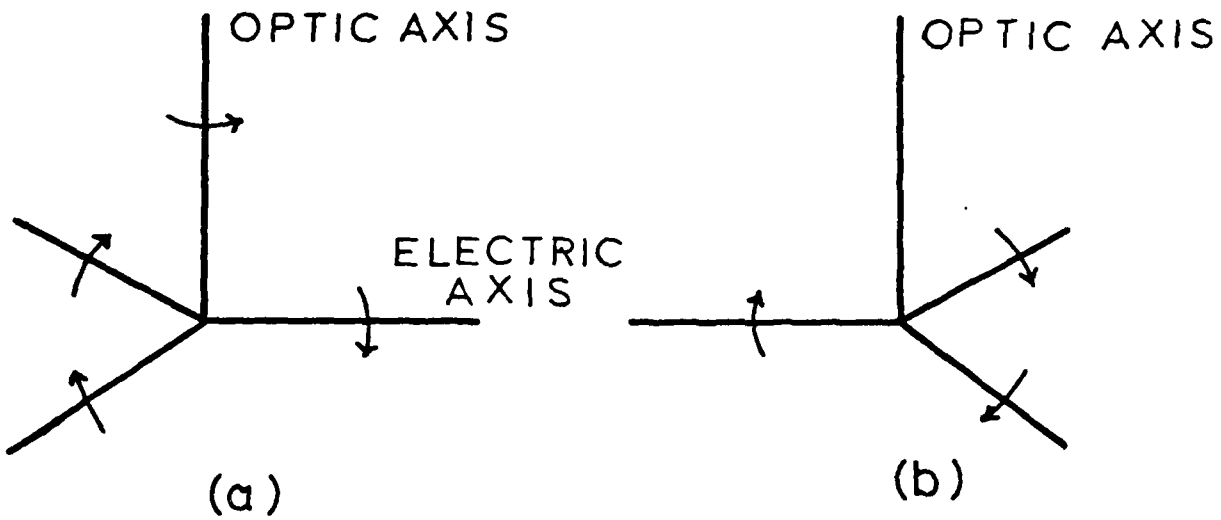

FIG. 5

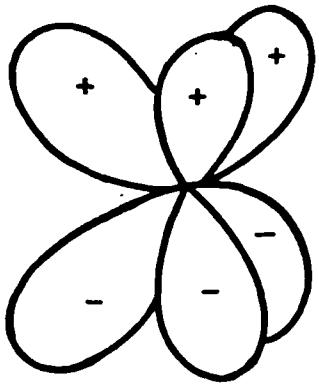

FIG. 6

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The paper is concerned with some underlying physical considerations which bear on the development of restrictions on the strain-energy function for an elastic material which may undergo finite deformations. Some comments are also made on the possible use of the strain-energy function at deformations for which a necessary condition for material stability is violated.

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