

Thermodynamic influences on stationary singular surfaces in materials with scalar internal variables

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STATIONARY singular surfaces may exist in materials with scalar internal variables. This paper shows that the jump of the second deformation gradient across such a surface behaves, under thermodynamic influences, as if the number of the scalar internal variables were increased by one. In other words, the entropy plays the same role as a scalar internal variable on the variation of the discontinuity. As a result, stationary singular surfaces may also exist in a thermoelastic material.

W materiałach ze skalarowymi zmiennymi wewnętrznymi mogą powstawać stacjonarne powierzchnie osobliwe. W pracy tej wykazuje się, że skok drugiego gradientu deformacji na takiej powierzchni zachowuje się pod wpływami termodynamicznymi, w ten sposób, jak gdyby liczba skalarowych zmiennych wewnętrznych zwiększyła się o jedność. Innymi słowy, entropia odgrywa przy zmianie nieciągłości taką samą rolę jak skalarowa zmienna wewnętrzna. W rezultacie okazuje się, że również w materiale termosprężystym mogą istnieć stacjonarne powierzchnie osobliwe.

В материалах со скалярными внутренними переменными могут возникать стационарные особые поверхности. В этой работе показывается, что скачок второго градиента деформации на такой поверхности ведётся под термодинамическими влияниями таким образом, как бы число скалярных внутренних переменных увеличилось на единицу. Другими словами, энтропия играет, при изменении разрыва, такую же самую роль, как скалярная внутренняя переменная. В результате оказывается, что тоже в термоупругом материале могут существовать стационарные особые поверхности.

1. Introduction

IN THE PREVIOUS paper [1] the author showed that there may exist stationary singular surfaces in a three-dimensional material with scalar internal variables. In this paper, thermodynamic influences on such stationary singular surfaces are studied. A thermodynamical theory of materials with internal variables have been developed in [2-4]. Propagating singular surfaces, i.e., acceleration waves in thermoelastic materials with internal variables, have been investigated in [5] and [6].

This paper employs the constitutive relations considered in [6], where the heat conduction is not taken into account and the internal energy is assumed to be a function of the deformation gradient, the entropy and an arbitrary number of scalar internal variables. In the next section the constitutive relations are given and a singular surface is defined. Section 3 proves that stationary singular surfaces may exist in the thermoelastic material no matter whether it has internal variables or not. In Sect. 4 the variation of the amplitudes of discontinuities across a stationary singular surface is analysed. It is shown that the jump of the second deformation gradient in a thermoelastic material with N scalar

internal variables behaves like the one in an elastic material with $N+1$ scalar internal variables. In other words, the entropy plays the same role as a scalar internal variable on the behaviour of the stationary singular surface.

2. Constitutive relations and definition of singular surfaces

The constitutive equations of nonconducting thermoelastic materials with N scalar internal variables are [2, §7, and 6]

$$(2.1) \quad \varepsilon = \hat{\varepsilon}(\mathbf{F}, \mathbf{a}, \eta),$$

$$(2.2) \quad \theta = \hat{\theta}(\mathbf{F}, \mathbf{a}, \eta) = \frac{\partial \hat{\varepsilon}}{\partial \eta}(\mathbf{F}, \mathbf{a}, \eta),$$

$$(2.3) \quad \mathbf{T} = \hat{\mathbf{T}}(\mathbf{F}, \mathbf{a}, \eta) = \rho \mathbf{F} \nabla_{\mathbf{F}} \hat{\varepsilon}(\mathbf{F}, \mathbf{a}, \eta)^T,$$

$$(2.4) \quad \mathbf{q} = \mathbf{0},$$

$$(2.5) \quad \dot{\mathbf{a}} = \boldsymbol{\psi}(\mathbf{F}, \mathbf{a}, \eta),$$

where ε is the internal energy density, η the entropy density, \mathbf{F} the deformation gradient, θ the absolute temperature, \mathbf{a} the vector of N scalar internal variables, \mathbf{T} the stress tensor, \mathbf{q} the heat flux and ρ the present density. We assume that $\boldsymbol{\psi}$ and $\hat{\varepsilon}$ are, respectively, once and twice continuously differentiable with respect to their arguments.

The balance equations are given by

$$(2.6) \quad \rho |\det \mathbf{F}| = \rho_*,$$

$$(2.7) \quad \operatorname{div} \mathbf{T} + \rho \mathbf{f} = \rho \dot{\mathbf{v}},$$

$$(2.8) \quad \mathbf{T} = \mathbf{T}^T,$$

$$(2.9) \quad \rho \dot{\varepsilon} = \operatorname{tr}(\mathbf{T} \dot{\mathbf{F}} \mathbf{F}^{-1}) - \operatorname{div} \mathbf{q} + \rho r,$$

where ρ_* is the constant density in the reference configuration, \mathbf{v} the velocity, \mathbf{f} the external body force density, and r the heat supply density. The dissipation inequality for the material without heat conduction is

$$(2.10) \quad \rho \dot{\eta} + \operatorname{div}(\mathbf{q}/\theta) - \rho r/\theta \geq 0.$$

Substituting Eqs. (2.1)–(2.5) into Eq. (2.9), we can rewrite the balance law of energy as

$$(2.11) \quad \dot{\eta} = \frac{1}{\theta} (\boldsymbol{\sigma} \cdot \boldsymbol{\psi} + r),$$

where \cdot means the inner product in the N -dimensional space of internal variables and

$$(2.12) \quad \boldsymbol{\sigma} \equiv -\nabla_{\mathbf{a}} \hat{\varepsilon}.$$

The dissipation inequality (2.10) is combined with Eqs. (2.4) and (2.11) to yield

$$(2.13) \quad \boldsymbol{\sigma} \cdot \boldsymbol{\psi} \geq 0.$$

It is convenient to represent the balance law of linear momentum (2.7) in terms of the first Piola–Kirchhoff stress tensor \mathbf{T}_* :

$$(2.14) \quad \operatorname{Div} \mathbf{T}_* + \rho_* \mathbf{f} = \rho_* \dot{\mathbf{v}},$$

where

$$(2.15) \quad \mathbf{T}_* \equiv |\det \mathbf{F}| \mathbf{T} \mathbf{F}^{-T}.$$

It follows from Eqs. (2.3), (2.6), (2.8) and (2.15) that

$$(2.16) \quad \mathbf{T}_* = \boldsymbol{\phi}(\mathbf{F}, \mathbf{a}, \eta) \equiv \varrho_* \nabla_{\mathbf{F}} \hat{\epsilon}(\mathbf{F}, \mathbf{a}, \eta).$$

We consider a plane singular surface S satisfying the following conditions:

(i) All of the deformations \mathbf{u} , \mathbf{v} , \mathbf{F} , \mathbf{a} and η are continuous with respect to the time and the coordinates.

(ii) The first derivatives of \mathbf{v} , \mathbf{F} , \mathbf{a} and η suffer finite jump discontinuities across S in a time interval.

(iii) Each of \mathbf{v} , \mathbf{F} , \mathbf{a} , η and the jumps of their first derivatives is uniform over S at any instant.

Let us call S simply a singular surface. We further assume that \mathbf{f} , \mathbf{r} and its spatial derivative are continuous with respect to the time and the coordinates, and that \mathbf{r} is uniform over S at any instant.

3. Existence of stationary singular surfaces

The first-order compatibility conditions for \mathbf{v} , \mathbf{F} , \mathbf{a} and η across a singular surface S are given by

$$(3.1) \quad [\dot{\mathbf{v}}^i] = U^2 e^i, \quad [F_j^i] = -U e^i n_j, \quad [F_{j,k}^i] = e^i n_j n_k,$$

$$(3.2) \quad [\dot{a}^\alpha] = -U b^\alpha, \quad [a_{,j}^\alpha] = b^\alpha n_j,$$

$$(3.3) \quad [\dot{\eta}] = -U c, \quad [\eta_{,j}] = c n_j,$$

where

$$(3.4) \quad e^i \equiv [F_{j,k}^i] n^j n^k, \quad b^\alpha \equiv [a_{,j}^\alpha] n^j, \quad c \equiv [\eta_{,j}] n^j,$$

and $[\cdot]$ denotes the jump of a quantity, \mathbf{n} a unit normal to S , U the speed of S in the \mathbf{n} direction. Here and henceforth Latin indices run from 1 to 3, and Greek ones from 1 to N . If $U = 0$, S is a stationary singular surface, and if $U \neq 0$, S is an acceleration wave.

Substituting Eq. (2.16)₁ into Eq. (2.14) yields

$$(3.5) \quad \frac{\partial \phi^{i,j}}{\partial F_Q^p} F_{Q,j}^p + \frac{\partial \phi^{i,j}}{\partial a^\alpha} a_{,j}^\alpha + \frac{\partial \phi^{i,j}}{\partial \eta} \eta_{,j} + \varrho_* f^i = \varrho_* \dot{v}^i.$$

Taking the jump of Eq. (3.5) across S and then using Eqs. (3.1)–(3.4), we obtain

$$(3.6) \quad (Q_p^i - \varrho_* U^2 \delta_p^i) e^p + R_\alpha^i b^\alpha + R_0^i c = 0,$$

where \mathbf{Q} is the acoustic tensor and

$$(3.7) \quad Q_p^i \equiv \frac{\partial \phi^{i,j}}{\partial F_Q^p} n_j n_Q, \quad R_\alpha^i \equiv \frac{\partial \phi^{i,j}}{\partial a^\alpha} n_j, \quad R_0^i \equiv \frac{\partial \phi^{i,j}}{\partial \eta} n_j.$$

Notice that Q_p^i , R_α^i and R_0^i depend on \mathbf{F} , \mathbf{a} and η together with \mathbf{n} . On the other hand, the jump relation of Eq. (2.5) across S becomes, by use of Eq. (3.2)₁,

$$(3.8) \quad U \mathbf{b} = \mathbf{0}.$$

It is easy to see from Eqs. (2.2) and (2.12) that θ and σ are continuous across S . From the assumption, r is also continuous across S , and therefore it follows from Eqs. (2.11) and (3.3)₁ that

$$(3.9) \quad Uc = 0.$$

The set of equations (3.6), (3.8) and (3.9) are the propagation conditions which determine U and the ratios among c and the components of \mathbf{e} and \mathbf{b} . In view of Eqs. (3.8) and (3.9) there are two possibilities: In the case when $U = 0$, S is a stationary singular surface, and \mathbf{b} and c need not vanish. Then Eq. (3.6) reduces to

$$(3.10) \quad Q_p^i e^p + R_\alpha^i b^\alpha + R_0^i c = 0.$$

In the other case when $\mathbf{b} = \mathbf{0}$ and $c = 0$, Eq. (3.6) becomes

$$(3.11) \quad (Q_p^i - \rho_\kappa U^2 \delta_p^i) e^p = 0.$$

Since \mathbf{e} should not vanish for S to be a singular surface, Eq. (3.11) implies that $\rho_\kappa U^2$ must be a real and nonnegative eigenvalue of \mathbf{Q} . The cases when the eigenvalue is zero and positive correspond, respectively, to a stationary singular surface and an acceleration wave. Thus, as well as in the case of elastic materials with scalar internal variables [1], there may exist two types of stationary singular surfaces.

As a special case, we consider a thermoelastic material without internal variables. To do so we may omit, in the constitutive relations and the equations derived from them, all the quantities associated with internal variables, i.e., \mathbf{a} , $\boldsymbol{\psi}$, $\boldsymbol{\sigma}$, \mathbf{b} and R_α^i . In consequence, we obtain the jump relations (3.6) without the term R_α^i and Eq. (3.9). Using an argument similar to the one above, it is found that *two types of stationary singular surfaces may also exist in the thermoelastic material.*

In what follows we assume that \mathbf{Q} does not have any null eigen value and consider the first type of stationary singular surfaces only. For later discussions it will be convenient to rewrite Eq. (3.10) as

$$(3.10) \quad Q_p^i e^p + R_\alpha^i b^{\alpha'} = 0,$$

where Greek indices with primes run from 0 to N , and

$$(3.12) \quad b^0 \equiv c.$$

4. Growth and decay of amplitudes of stationary singular surfaces

In this section we study the variation of the discontinuities \mathbf{e} , \mathbf{b} and c across a stationary singular surface S . The second-order compatibility conditions for \mathbf{a} and η across S required for the analysis are

$$(4.1) \quad [\dot{a}^{\alpha,j}] = \left(\frac{\delta}{\delta t} b^\alpha \right) n_j,$$

$$(4.2) \quad [\dot{\eta}_{,j}] = \left(\frac{\delta}{\delta t} c \right) n_j,$$

where $\delta/\delta t$ means the time differentiation of a jump quantity. Differentiating Eqs. (2.5) and (2.11) with respect to X^J , we get respectively

$$(4.3) \quad \dot{a}^{\alpha}_{,J} = \frac{\partial \psi^{\alpha}}{\partial F^p_Q} F^p_{Q,J} + \frac{\partial \psi^{\alpha}}{\partial a^{\beta}} a^{\beta}_{,J} + \frac{\partial \psi^{\alpha}}{\partial \eta} \eta_{,J},$$

$$(4.4) \quad \dot{\eta}_{,J} = -\frac{1}{\theta^2} (\sigma_{\alpha} \psi^{\alpha} + r) \theta_{,J} + \frac{1}{\theta} (\sigma_{\alpha, J} \psi^{\alpha} + \sigma_{\alpha} \psi^{\alpha}_{,J} + r_{,J}).$$

By the assumption σ , ψ and $\hat{\theta}$ are smooth functions of F , a and η , so that Eq. (4.4) may be transformed as

$$(4.5) \quad \dot{\eta}_{,J} = V_i^K F^i_{K,J} + W_{\alpha} a^{\alpha}_{,J} + Z \eta_{,J} + \frac{1}{\theta} r_{,J},$$

where

$$(4.6) \quad V_i^K \equiv -\frac{1}{\theta^2} (\sigma_{\alpha} \psi^{\alpha} + r) \frac{\partial \hat{\theta}}{\partial F^i_K} + \frac{1}{\theta} \frac{\partial \sigma_{\alpha}}{\partial F^i_K} \psi^{\alpha} + \frac{1}{\theta} \sigma_{\alpha} \frac{\partial \psi^{\alpha}}{\partial F^i_K},$$

$$(4.7) \quad W_{\alpha} \equiv -\frac{1}{\theta^2} (\sigma_{\beta} \psi^{\beta} + r) \frac{\partial \hat{\theta}}{\partial a^{\alpha}} + \frac{1}{\theta} \frac{\partial \sigma_{\beta}}{\partial a^{\alpha}} \psi^{\beta} + \frac{1}{\theta} \sigma_{\beta} \frac{\partial \psi^{\beta}}{\partial a^{\alpha}},$$

$$(4.8) \quad Z \equiv -\frac{1}{\theta^2} (\sigma_{\alpha} \psi^{\alpha} + r) \frac{\partial \hat{\theta}}{\partial \eta} + \frac{1}{\theta} \frac{\partial \sigma_{\alpha}}{\partial \eta} \psi^{\alpha} + \frac{1}{\theta} \sigma_{\alpha} \frac{\partial \psi^{\alpha}}{\partial \eta}.$$

Taking the jump relations of Eqs. (4.3) and (4.5) across S by use of Eqs. (3.1)₃, (3.2)₃, (3.3)₃, (4.1) and (4.2), and then multiplying the results by n^J , we get respectively

$$(4.9) \quad \frac{\delta}{\delta t} b^{\alpha} = A_p^{\alpha} e^p + B_{\beta}^{\alpha} b^{\beta} + B_0^{\alpha} c,$$

$$(4.10) \quad \frac{\delta}{\delta t} c = A_p^0 e^p + B_{\beta}^0 b^{\beta} + B_0^0 c,$$

where

$$(4.11) \quad A_p^{\alpha} \equiv \frac{\partial \psi^{\alpha}}{\partial F^p_Q} n_Q, \quad A_p^0 \equiv V_p^K n_K,$$

$$(4.12) \quad B_{\beta}^{\alpha} \equiv \frac{\partial \psi^{\alpha}}{\partial a^{\beta}}, \quad B_0^{\alpha} \equiv \frac{\partial \psi^{\alpha}}{\partial \eta},$$

$$(4.13) \quad B_{\beta}^0 \equiv W_{\beta}, \quad B_0^0 \equiv Z.$$

Here note that by the assumption $r_{,J}$ is continuous across S . By use of Eq. (3.12) we can rewrite (4.9) and (4.10) as the single equation

$$(4.14) \quad \frac{\delta}{\delta t} b^{\alpha'} = A_p^{\alpha'} e^p + B_{\beta'}^{\alpha'} b^{\beta'},$$

where recall that Greek indices with primes run from 0 to N . Comparing Eqs. (3.10') and (4.14) with Eqs. (2.11) and (3.5) in [1], we see that the jump associated with the gradient of the entropy plays the same role as the one of a scalar internal variable and that the amplitude equations take the same form as those for the elastic material with $N+1$

scalar internal variables. Thus we can apply the results of the preceding paper to analyse the variation of the amplitudes. Eliminating e from Eqs. (3.10)' and (4.14), we obtain a system of linear differential equations for $b^{\alpha'}$:

$$(4.15) \quad \frac{\delta}{\delta t} b^{\alpha'} = C_{\beta'}^{\alpha'} b^{\beta'},$$

where

$$(4.16) \quad C_{\beta'}^{\alpha'} = -A_p^{\alpha'} Q_i^{-1p} R_{\beta'}^i + B_{\beta'}^{\alpha'}.$$

At the stationary singular surface S , F , a , η and r may depend on the time, and hence C is, in general, a matrix-valued function of the time. Then Eq. (4.15) can be solved as

$$(4.17) \quad b^{\alpha'}(t) = P_{\beta'}^{\alpha'}(t) b_0^{\beta'},$$

where $b_0^{\beta'}$ are constants and

$$(4.18) \quad P_{\beta'}^{\alpha'}(t) \equiv \delta_{\beta'}^{\alpha'} + \int_{t_0}^t C_{\beta'}^{\alpha'}(\tau) d\tau + \int_{t_0}^t C_{\gamma'}^{\alpha'}(\tau_1) \int_{t_0}^{\tau_1} C_{\beta'}^{\gamma'}(\tau_2) d\tau_2 d\tau_1 + \dots$$

Substituting Eq. (4.17) into Eq. (3.10)' and then multiplying the result by Q_i^{-1a} , we get

$$(4.19) \quad e^a = -Q_i^{-1a} R_{\alpha'}^i P_{\beta'}^{\alpha'} b_0^{\beta'}.$$

Applying Theorem 1 in [1] to this case, we have

THEOREM 1. *If Q does not have any null eigen value for every $t \geq t_0$, e , b and c are bounded for each $t \geq t_0$.*

Let us consider a special case where F , a , η and r are constant in time at S . Then from Eqs. (4.6)–(4.8), (4.11)–(4.13) and (4.16) C reduces to a constant $(N+1) \times (N+1)$ matrix C_0 , and Theorem 2 in [1] implies

THEOREM 2. *Suppose that F , a , η are constant in time at S and that Q does not have any null eigenvalue. If the real parts of all eigenvalues of C_0 are negative, e , b and c tend to zeros as $t \rightarrow \infty$.*

Next suppose that the number of the scalar internal variables is unknown and that we can determine the time derivatives $e_i \equiv e^{(i)p}(t_0)$ ($i = 0, 1, \dots, L$) of a component e^p at a time t_0 by observing the S . Define for each $n = 1, 2, \dots, L$

$$(4.20) \quad G_n \equiv \begin{vmatrix} e_0 & e_1 & \dots & e_{n-1} \\ e_1 & e_2 & \dots & e_n \\ \dots & \dots & \dots & \dots \\ e_{L-n} & e_{L-n+1} & \dots & e_{L-1} \end{vmatrix},$$

$$(4.21) \quad H_n \equiv \begin{vmatrix} e_0 & e_1 & \dots & e_n \\ e_1 & e_2 & \dots & e_{n+1} \\ \dots & \dots & \dots & \dots \\ e_{L-n} & e_{L-n+1} & \dots & e_L \end{vmatrix}.$$

Then from Theorem 3 in [1], we have for the thermoelastic material with scalar internal variables

THEOREM 3. *If N' is the maximum integer such that $\text{rank } G_n \neq \text{rank } H_n$ for every $n \leq N'$, then the number of the internal variables is larger than $N' - 1$.*

It should be noted that unlike the case of elastic materials with scalar internal variables \mathbf{C} does not reduce to a constant matrix when the constitutive functions $\hat{\theta}$, σ , ϕ and ψ , are linear. In fact, \mathbf{C} contains the terms $1/\theta^2$, $1/\theta$ and r , where refer to Eqs. (4.6)–(4.8), (4.11)–(4.13) and (4.16).

References

1. E. MATSUMOTO, *Stationary singular surfaces in materials with scalar internal variables*, Arch. Mech., **34**, 4, 1982.
2. B. D. COLEMAN, M. E. GURTIN, *Thermodynamics with internal state variables*, J. Chem. Phys., **47**, 597–613, 1967.
3. R. M. BOWEN, *Thermochemistry of reacting materials*, J. Chem. Phys., **49**, 1625–1637, 1968; **50**, 4601–4602, 1969.
4. R. M. BOWEN, *On the stoichiometry of chemically reacting materials*, Arch. Rational Mech. Anal., **29**, 114–124, 1968.
5. R. M. BOWEN, C. C. WANG, *Thermodynamic influences on acceleration waves in inhomogeneous isotropic elastic bodies with internal state variables*, Arch. Rational Mech. Anal., **41**, 287–318, 1971.
6. R. M. BOWEN, P. J. CHEN, *Acceleration waves in anisotropic thermoelastic materials with internal state variables*, Acta Mech., **15**, 95–104, 1972.

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