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THERMODYNAMIC AND ENERGETIC FORCES IN THERMOELASTICITY

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Abstract—Crack driving forces for thermoelasticity are derived on the basis of the general framework of Thermodynamics of Irreversible Processes. It is demonstrated that the thermodynamic forces are distinct from conventional energetic forces. Relationships between the two types of forces are investigated and a possible experimental examination as to whether thermodynamic or energetic forces might be responsible for crack propagation is discussed.

1. INTRODUCTION

Energetic forces are introduced to characterize causes which drive cracks and other defects in solids[1]. These forces are defined as partial derivatives of potential energy with respect to corresponding defect configuration parameters.

Usually fracture is an irreversible process which is often coupled with other irreversible physicochemical processes like phase and chemical transformations, heat and mass transfer, etc. Thermodynamics of irreversible processes (TIP) offers a general framework to study these phenomena, in particular, by introducing the thermodynamic forces. It is demonstrated below that thermodynamic forces are distinct from conventional energetic forces like the J-integral.

In this paper thermodynamic and energetic forces for thermoelasticity are derived following the thermodynamic approach[2]. Relationships between the two types of forces are investigated and a possible experimental examination as to whether thermodynamic or energetic forces might be responsible for a crack propagation, is discussed.

2. THERMODYNAMIC CONSIDERATION

Crack growth is usually preceded and accompanied by damage. In this paper we identify damage as a system of material inhomogeneities, and damage nucleation and growth as a material transformation. Damage, in general, can be characterized by its density and orientation. We assume, for simplicity, that the orientation of inhomogeneities with respect to the crack does not vary in a process of crack growth and accompanying damage propagation. Therefore, the scalar damage density is incorporated as the only thermodynamic state parameter characterizing damage.

The stress tensor σ_{ij} and the absolute temperature T conventionally constitute a set of state parameters for thermoelasticity. This set, extended by the damaged parameter ρ, is chosen as a list of state parameters for the damaged thermoelastic medium:

$$\{\sigma_{ij}, T, \rho\}. \tag{1}$$

In what follows we derive the thermodynamic forces associated with damage.

The local energy balance is conventionally taken as

$$\dot{u} = \sigma_{ij}\dot{\varepsilon}_{ij} - \partial_k j_k^Q. \tag{2}$$

Here u stands for the rate of internal energy density, $\dot{\varepsilon}_{ij}$ is the strain rate tensor, the product $\sigma_{ij}\dot{\varepsilon}_{ij}$ represents the rate of work density, j_k^Q stands for the heat flux, and the usual summation convention on repeated indices is employed.

It is convenient to express the internal energy density u in term of Gibbs' potential density g and the entropy density s:

$$u = g + Ts + \sigma_{ij}\varepsilon_{ij}. \tag{3}$$

Here, ε_{ij} is the total strain tensor component.

The entropy production $\dot{s}_i$ introduced in TIP is the most important characteristic of irreversible processes. It is defined as a portion of the total entropy density rate $\dot{s}$

$$\dot{s}_i = \dot{s} - \dot{s}_e \tag{4}$$

with $\dot{s}_e = -\partial_k[(1/T)j_k^Q]$ to be the entropy density rate due to heat exchange (for a closed system).

Employing the energy balance (2), decomposition of the internal energy density (3), and definition of the entropy production (4) we arrive at

$$\dot{s}_i = -\frac{1}{T}\left(\dot{g} + s\dot{T} + \varepsilon_{ij}\dot{\sigma}_{ij} + j_k^Q \frac{\partial_k T}{T}\right). \tag{5}$$

In conventional thermoelasticity, the Gibbs' potential density g, often designated as the thermoelastic potential energy density π, is expressed as a Taylor's decomposition with respect to the state parameters σ_{ij} and T. The coefficients of decomposition represent material properties such as elastic compliances, thermal expansion coefficient, etc., and the first term of the decomposition represents the reference level of g.

For the damaged thermoelastic medium, the rate of Gibbs' potential density $\dot{g}$ is affected by damage growth $\dot{\rho}$ in two ways, through changes in (i) the reference level and (ii) the material property coefficients included in π. Hence,

$$\dot{g}(\sigma_{ij}, T, \rho) = \gamma(\sigma_{ij}, T)\dot{\rho} + \dot{\pi}(\sigma_{ij}, T, \rho). \tag{6}$$

Here, γ is the difference between Gibbs' potential densities in undamaged and damaged states per unit damage density; and π is taken in the same form as in conventional thermoelasticity, but with the material property coefficients being functions of the damage parameter ρ.

The assumption of local equilibrium, conventional in TIP, yields the thermoelastic constitutive equations:

$$\left.\frac{\partial \pi}{\partial T}\right|_{\rho}^{\sigma_{ij}} = -s, \tag{7}$$

$$\left.\frac{\partial \pi}{\partial \sigma_{ij}}\right|_{\rho}^{T} = -\varepsilon_{ij}. \tag{8}$$

Accounting for (6)–(8) the local entropy production (5) takes the form:

$$\dot{s}_i = -\frac{1}{T}\left(\gamma + \frac{\partial \pi}{\partial \rho}\right)\dot{\rho} - \frac{\partial_k T}{T^2} j_k^Q. \tag{9}$$

In TIP, entropy production is conventionally presented as a bilinear form of generalized fluxes and reciprocal thermodynamic forces, such as j_k^Q and $-\partial_k T/T^2$ for heat transfer. For the rate of damage density $\dot{\rho}$, taken as a flux, the reciprocal force is $-(1/T)[\gamma + (\partial\pi/\partial\rho)]$.

3. CRACK LAYER APPROACH

A system of a crack and its surrounding damage is designated as a crack layer (CL) [2]. The part of the CL within which the rate of damage accumulation is positive ($\dot{\rho} > 0$) is defined as an active zone. For a small active zone, the CL theory models fracture propagation as active zone movements: translation, rotation, isotropic expansion, and distortion. There are thermodynamic forces corresponding to each of these elementary movements. In this paper we consider translational and expansional forces only. They can be identified based on global entropy production due to CL translation and expansion.

The global entropy production is the integral of (9) over the entire volume of a solid:

$$S_i^{\text{global}} = \int_V \dot{s}_i \, \mathrm{d}V = -\int_V \frac{\gamma}{T}\dot{\rho} \, \mathrm{d}V - \int_V \frac{\partial \pi}{\partial \rho}\frac{\dot{\rho}}{T} \, \mathrm{d}V - \int_V \frac{\partial_k T}{T^2} j_k^Q \, \mathrm{d}V. \tag{10}$$

The first two integrals on the r.h.s. of (10) are reduced to those over the active zone V_A since $\dot{\rho}$ is nonzero only within this domain and they represent the global entropy production due to damage growth. The first integral is associated with the energy consumed by material transformation from an undamaged into a damaged state such as craze or new surface formation. It reflects the resistance to CL propagation. The second integral evidently represents the entropy production associated with the potential energy release rate, and is defined as the impellent of CL. The last integral in (10) conventionally reflects the entropy rate due to heat transfer.

It is assumed that the active zone moves maintaining a self-similar distribution of damage such that the rate of damage density $\dot{\rho}$ at a given point **x**, in an Euler system of coordinates, can be expressed as

$$\dot{\rho}(x) = -V_k(\xi) \cdot \partial_k \rho(\xi) \tag{11}$$

where $\boldsymbol{\xi}$ is a position vector in the movable system of Cartesian coordinates with the origin at the crack tip and the 1-axis chosen along the tangent to the crack trajectories, $V_k(\xi)$ is the kth component of the velocity vector. Reducing the general motion of the active zone to the 2D translation $\dot{l}$ and isotropic expansion $\dot{e}$, the velocity is

$$V_k(\xi) = \dot{l}\delta_{1k} + \dot{e}\xi_k, \tag{12}$$

provided $i,k = 1, 2$ and δ_{ik} is the Kronecker symbol.

It should be noted that the rate of the active zone translation $\dot{l}$ coincides with the rate of crack growth.

The damage density rate $\dot{\rho}$ (11) with (12) becomes

$$\dot{\rho}(x) = -\dot{l}\partial_1 \rho(\xi) - \dot{e}\xi_k \, \partial_k \rho(\xi). \tag{13}$$

Upon substitution of (13) into (10) we write

$$S_i^{\text{global}} = \dot{l}X_1 + \dot{e}X^{\text{exp}} - \int_V j_k^Q \frac{\partial_k T}{T^2} \mathrm{d}V. \tag{14}$$

Here, $\dot{l}$ and $\dot{e}$ are considered to be generalized fluxes which stand for translation and expansion of the active zone, respectively; X_1 and X^{exp} are reciprocal thermodynamic forces:

$$X_1 = I_1 - R_1 \tag{15}$$

$$X^{\text{exp}} = I^{\text{exp}} - R^{\text{exp}}. \tag{16}$$

In the above expressions R_1, and R^{exp} represent the resistance to active zone translation and expansion. I_1 and $I^{\exp}$ are defined as translational and expansional impellents. From (10) and (13) we obtain:

$$I_1 = \int_{V_A} \frac{1}{T}\frac{\partial \pi}{\partial \rho}\partial_1 \rho \,\mathrm{d}V \tag{17}$$

$$I^{\exp} = \int_{V_A} \frac{1}{T}\frac{\partial \pi}{\partial \rho}\xi_k \,\partial_k \rho \,\mathrm{d}V. \tag{18}$$

4. IMPELLENT FORCES IN THERMOELASTICITY

The translational impellent

For a homogeneous medium the density of elastic potential energy π is a function of the state parameters and does not depend on coordinates explicitly:

$$\pi = \pi[\sigma_{ij}(\xi), T(\xi), \rho(\xi)]. \tag{19}$$

Consequently,

$$\frac{\partial \pi}{\partial \rho}\partial_k \rho = \partial_k \pi - \frac{\partial \pi}{\partial \sigma_{ij}}\partial_k \sigma_{ij} - \frac{\partial \pi}{\partial T}\partial_k T, \tag{20}$$

where, for a two-dimensional case, i, j and $k = 1, 2$.

Using constitutive eqns (7) and (8), (20) can be rewritten as

$$\frac{\partial \pi}{\partial \rho}\partial_k \rho = \partial_k \pi + \varepsilon_{ij}\,\partial_k \sigma_{ij} + s\,\partial_k T. \tag{21}$$

Elastic potential energy density is defined as

$$\pi = f - \sigma_{ij}\varepsilon_{ij}, \tag{22}$$

where f represents the strain energy density which is conventionally expressed in thermoelasticity as follows:

$$f = \tfrac{1}{2}\sigma_{ij}[u_{i,j} - \alpha_{ij}(T - T_0)]. \tag{23}$$

The value α_{ij} is a coefficient of thermal expansion, T_0 is the absolute temperature for the natural state when the strain is zero everywhere, and u_i is a displacement component.

Constitutive relation (7) with (22) and (23) gives rise to

$$s = \alpha_{ij}\sigma_{ij}. \tag{24}$$

Upon substitution of (21), (22) and (24) into (17) and accounting for equilibrium equations

$$\sigma_{ij,j} = 0, \tag{25}$$

I_1 can be rewritten as

$$I_1 = \int_{V_A} \frac{1}{T}\,[\partial_1 f - \partial_j(\sigma_{ij}\beta_{i1})]\,\mathrm{d}V. \tag{26}$$

Here, β_{ij} is an elastic distortion defined as the difference between the total distortion $u_{i,j}$ and the thermal $\alpha_{ij}(T - T_0)$. Then, the total strain $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$.

Employing Gauss' theorem we finally arrive at

$$I_1 = \int_{\partial V_A} \frac{1}{T}(f \cdot n_1 - \sigma_{ij} n_j \beta_{i1})\, \mathrm{d}\Gamma - \int_{V_A} \frac{1}{T^2}(f \cdot T_{,1} - \sigma_{ij}\beta_{i1} T_{,j})\, \mathrm{d}V. \tag{27}$$

Here n_j is the jth component of the unit outward normal to an integration path dV_A.

The expansional impellent

Upon application of the technique used above, the expansional impellent I^{exp} results in the following form:

$$I^{\mathrm{exp}} = \int_{V_A} \frac{1}{T}[\partial_k(\xi_k f) - \partial_j(\xi_k \sigma_{ij} \beta_{ik})]\, \mathrm{d}V. \tag{28}$$

Applying Gauss' theorem to (28) we have

$$I^{\mathrm{exp}} = \int_{\partial V} \frac{1}{T}(\xi_k n_k f - \sigma_{ij}\beta_{ik}\xi_k n_j)\, \mathrm{d}\Gamma - \int_{V_A} \frac{1}{T^2}(f \xi_k\, \partial_k T - \sigma_{ij} T_{,j} \xi_k \beta_{ik})\, \mathrm{d}V. \tag{29}$$

The area integrals in (27) and (29) cannot be, in general, converted into line integrals.

The path integrals in (27) and (29) resemble the well-known elastic J_1- and M-integrals. Similitude between I_1 and I^{exp} on one side, and J_1 and M on another reflects a relationship between thermodynamic and energetic forces which is discussed below.

5. ENERGETIC FORCES IN THERMOELASTICITY

A number of papers on evaluation of the energy release rate for thermoelasticity and the corresponding J-integral have been published since 1978. Two main formalisms have been developed to derive the energetic forces in elasticity. The first is based on direct calculation of the potential energy rate with respect to crack length; the second makes use of Lagrangian formalism. The formalisms have been extended for thermoelasticity by several authors[3–8]. The problem is discussed in Refs. [9–11]. A brief review of the results can be found in Refs. [7, 8].

To derive the energetic forces in this section we follow the formalism of Ref. [2] extended to thermoelasticity in Ref. [8].

Let us consider now the rate of potential energy $\dot{P}$ due to damage growth

$$\dot{P} = \int_V \frac{\partial \pi}{\partial \rho} \dot{\rho}\, \mathrm{d}V. \tag{30}$$

Upon substitution of (13) into (30) we conclude that P can be expressed through translational and expansional energetic forces:

$$\dot{P} = -\dot{l} J_1 - \dot{e} M, \tag{31}$$

where the translational energetic force is

$$J_1 = -\frac{\partial P}{\partial l} = \int_{V_A} \frac{\partial \pi}{\partial \rho} \partial_1 \rho\, \mathrm{d}V \tag{32}$$

and expansional

$$M = -\frac{\partial P}{\partial e} = \int_{V_A} \frac{\partial \pi}{\partial \rho} \xi_k\, \partial_k \rho\, \mathrm{d}V. \tag{33}$$

Upon application of the same technique as in the previous section, the integrals (32) and (33) become path integrals:

$$J_1 = \int_{\partial V_A} [f n_1 - \sigma_{ij} n_j \beta_{i1}] \,\mathrm{d}\Gamma \tag{34}$$

$$M = \int_{\partial V_A} [f \xi_k n_k - \sigma_{ij} n_j \xi_k \beta_{ik}] \,\mathrm{d}\Gamma. \tag{35}$$

These integrals repeat those in elasticity, except for employing distortion β_{ij} instead of $u_{i,j}$. In essence (34) and (35) are the same as those obtained earlier in Ref. [8], although presented in the different form. In Ref. [8] J_1 and M are expressed by means of the total displacement vector and consist of both the path and the area integrals.

Since the integrands in (34) and (35) are obtained from divergent forms and $\dot{\rho} = 0$ everywhere outside V_A, the J_1- and M-integrals are path invariant if $\partial_k T = 0$ in this domain also. Otherwise, path independence is not guaranteed, although J and M still represent the corresponding energetic forces on the whole domain inside the chosen path.

6. DISCUSSION

To illustrate the relationships between thermodynamic and energetic forces we consider the translational impellent I_1 and the energy release rate J_1.

The thermodynamic impellent I_1 has been derived as

$$I_1 = \int_{\partial V_A} \frac{f n_1 - \sigma_{ij} n_j \beta_{i1}}{T} - \int_{V_A} \frac{f \cdot T_{,1} - T_{,j} \sigma_{ij} \beta_{i1}}{T^2} \,\mathrm{d}V. \tag{27}$$

The energetic force is given by the J-integral in eqn (34). Here, we analyze the relationship between the two for certain special cases.

An infinitesimal active zone

By shrinking the active zone V_A onto the crack tip, we derive the I_1-integral for an infinitesimal active zone. In the vicinity of the crack tip, the asymptotic behavior of thermoelastic stress–strain fields repeats that for an elastic case. Hence, the singularity in f and $\sigma_{ij}\beta_{i1}$ is of the order of r^{-1}. It can be shown[12] that at the crack tip there is no singularity in the temperature field and the order of singularity in temperature gradient does not exceed that of $r^{-1/2}$, except in the case when a heat source is located at the crack tip. Therefore, when the active zone V_A is shrinking onto the crack tip, the area integral in eqn (27) vanishes and the temperature approaches its value at the crack tip, $T(0)$. After taking the limit described above, (27) and (34) lead to

$$I_1 = \frac{J_1}{T(0)}. \tag{36}$$

The integral J_1 can be computed by the conventional recipe.

The isothermal condition

For an isothermal condition, i.e. $\partial_k T = 0$, the area integral in (27) vanishes and it reduces to

$$I_1 = \frac{1}{T} J_1, \tag{37}$$

provided that eqn (34) is taken into account. The temperature T is uniform but not necessarily equal to the temperature T_0 of the normal state. Therefore, the thermoelastic J_1-integral is distinguished from pure elastic J_1^{el} and depends on the temperature differential $T-T_0$. At the normal state, i.e. in pure elasticity, the impellent is

$$I_1^{\mathrm{el}} = \frac{J_1^{\mathrm{el}}}{T_0} \tag{38}$$

and, thus in general, differs from that of eqn (37).

Small temperature variations

It should be noted that in linear thermoelasticity, the dimensionless temperature differential $\theta = (T-T_0)/T_0$ is assumed to be small, so that terms containing θ^2 can be neglected. With this approximation eqn (26) can be replaced by the following:

$$I_1 = \frac{1}{T_0} J_1(\theta) - \frac{1}{T_0} \int_{V_A} \theta[\partial_1 f - \sigma_{ij}(\partial_{ij}\beta_{i1})] \, \mathrm{d}V. \tag{39}$$

Since the integral in eqn (39) has the same sign as θ, it is evident the impellent can be greater or smaller then $J_1(\theta)/T_0$. I_1 can also be equal to J_1/T_0. The area integral in eqn (39) vanishes, for instance, when heat flow is uniform at infinity provided that the steady state temperature is disturbed by an insulated crack with the circular active zone centered at the crack tip.

Relationships analogous to eqns (36)–(39) are valid also for the thermodynamic and energetic expansional forces I^{exp} and M.

7. CONCLUDING REMARKS

Thermodynamic and energetic forces have been derived for thermoelasticity. Which is the true force driving a crack? Essentially different from each other, they are both candidates. One can resolve this dilemma by setting up an appropriate experimental examination based on the difference in temperature dependencies of the thermodynamic and energetic forces. One of the forces should be isolated from influencing crack propagation by keeping it constant. The test thus conducted would reveal the dependence of the crack velocity on the variation of the other force. Then we could identify the true force based on its one-to-one correspondence with the crack growth rate.

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