

Thermodynamics of translational crack layer propagation*

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Recognizing that fracture in many materials propagates as a crack preceded by intensive damage, a theory is presented to model the crack and the preceding damage as a single thermodynamic entity, i.e., a crack layer (CL). The active zone of the CL may propagate by translational, rotational, expansional and/or distortional movements. Concepts of irreversible thermodynamics are employed to derive the law of CL propagation by translational mode as:

$$\dot{l} = \frac{\beta J_1 \langle d \rangle}{\gamma^* R_1 - J_1}$$

where \dot{l} is the rate of CL translation, β is a dissipative coefficient, J_1 is the energy release rate, $\langle d \rangle$ is a characteristic size of the active zone, γ^* is the specific enthalpy of damage and R_1 is the translational resistance moment. This expression describes the entire history of CL propagation. Experimental results on fatigue crack propagation in polystyrene are in good agreement with the proposed formalism.

1. Introduction

Fracture of solids, polymers are no exception, occurs as a sequence of molecular processes leading to microscopic (local) damage. Accumulation of local damage gives rise to a macroscopic crack which propagates; first in a slow fashion, then critically (avalanche-like) causing ultimate failure. Efforts addressing long term strength of materials generally extend into three main directions: (1) phenomenological theories of local long term strength, (2) studies of crack propagation, and (3) statistical approach to failure. A theory unifying these three facets is being advanced at present by Chudnovsky and coworkers [1–8]. The theory recognizes a representative volume of the material as the basis for property determination at a point within the continuum. The size of the representative volume which must be large in comparison with the elementary substructure is determined from conditions of statistical homogeneity [9]. In this respect, the theory identifies fracture events within three interrelated scales.

Considering polymers as an illustrative example, the accumulation of intra and interchain motion, and chain scission may be conceived as sub-microscopic events. The accumulation of submicroscopic events to a critical level leads to microscopic damage. Macroscopic cracks appear as a result of the accumulation of microscopic damage to a critical level. The crack(s) propagates first in a quasistatic fashion until a stage is reached where catastrophic failure is experienced due to global instability.

Present experimental techniques provide useful qualitative information documenting the evolution of submicroscopic events giving rise to microscopic damage. It is within the microscale (10^{-6} – 10^{-4} m) where damage evolution can be characterized quantitatively with a reasonable degree of accuracy. Accordingly, information can be obtained to test ideas modeling crack initiation and propagation. Having this in mind, we proceed to describe the crack layer model for crack propagation in polymers.

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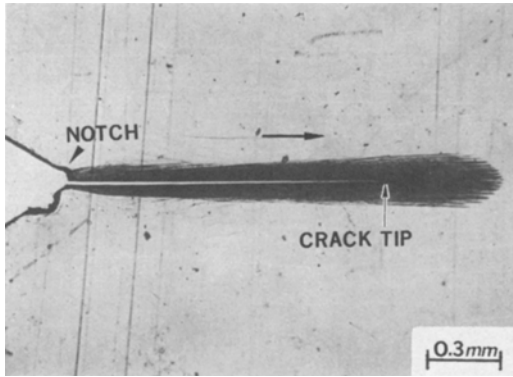


Figure 1 An optical micrograph of a SEN polystyrene specimen under fatigue loading. The propagating crack is preceded and surrounded with intensive crazing [8].

2. The crack layer concept

Microscopic damage accumulation to a critical level is always a precursor of crack initiation, even in the presence of a notch [10, 11]. Once initiated, the crack grows surrounded and preceded by a damage zone. The latter consists of structural transformations such as crazes, shear bands, voids, crystallinity changes, etc. Although the space within which such transformations disseminate can be very small compared with crack length, the energy expended on it could be orders of magnitude higher than that expended on the creation of crack “surfaces” [4, 12]. For example, Fig. 1 exhibits a layer of extensive crazing accompanying fatigue crack propagation in polystyrene [7]. Similar features of fracture propagation have been observed recently in various materials [4, 6, 10, 13–15]. A rational model of fracture propagation has to account for the fracture phenomenon as observed. Two complementary procedures should be followed. One is to model the stress–strain field due to the interaction of the main crack and multiple microcracks (crazes). The second is a thermodynamic approach which describes the system in terms of integral damage characteristics. Recent reports [5, 16] describe early results of elastic crack damage interaction. The general thermodynamic framework of the crack layer theory is presented in [17]. In the present paper, the discussion is limited to a thermodynamic treatment of crack layer propagation by translational mode. Crack layer propagation in polystyrene [11] is used as an illustrative example.

2.1. Damage density

In our model, damage is defined as discontinuities

such as microcracks, crazes, shear bands, etc. Such discontinuities can be visualized as two dimensional defects and thus be characterized by their middle surfaces. Specifically, we use the total area of middle surfaces of discontinuities within a unit volume as damage density, ρ , with the dimension m^2m^{-3} . For example, the craze density in the vicinity of the main crack has been directly evaluated from optical micrographs of thinned polypropylene samples [6]. A more complete description of damage requires an additional parameter characterizing orientation [17]. In this paper, since we consider rectilinear crack propagation where no change in damage orientation occurs, ρ suffices for damage characterization.

2.2. Definition of the crack layer

A system consisting of a crack and surrounding damage is considered as a macroscopic entity; that is a crack layer, (CL), (Fig. 2). This is a layer of transformed (damaged) material which propagates into the initial material. The front zone of the CL within which damage accumulation is non zero ($\rho > 0$; $\dot{\rho} > 0$) is defined as the active zone. At temperatures well below the glass transition T_g , the rate of damage-change (further growth or healing) under unloading conditions is negligible. Thus, a wake zone ($\rho > 0$; $\dot{\rho} = 0$) appears as a trace of the active zone propagation. The active zone is confined by a leading edge, ($\Gamma^{(l)}$), and a trailing edge, ($\Gamma^{(t)}$), (Fig. 2). Motion of the active zone, in the general sense, can be resolved into the following elementary movements: translation, rotation, isotropic expansion, and distortion (shape changes). Usually, the size of the active zone is small with respect to the crack length, therefore affine deformation of the active zone can reasonably approximate the actual evolution of damage. Accordingly, the rates of translation \dot{l} , rotation $\dot{\omega}$, isotropic expansion $\dot{\epsilon}$, and distortion $\dot{\mathbf{d}}$,

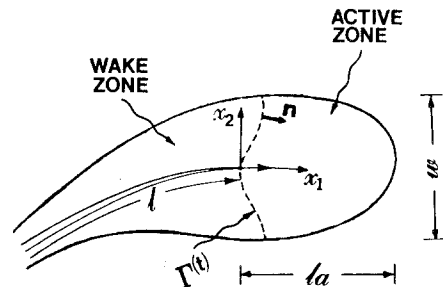


Figure 2 A schematic illustration of a crack layer in an infinite plane.

are considered as thermodynamic fluxes. The law of CL propagation is thus established by relating the fluxes to the reciprocal forces (causes) within the framework of irreversible thermodynamics.

3. Thermodynamic relations

We consider fracture propagation as a thermodynamically irreversible process. For such a process, the principle of extremal entropy production usually substitutes the variational principle of classical thermodynamics. The total entropy change of a solid containing a CL is given by

$$\dot{S}^{\text{TOT}} = \dot{S}_i + \dot{S}_e \quad (1)$$

where \dot{S}_i is the entropy production due to CL propagation and other dissipative processes, and \dot{S}_e is the rate of entropy change due to exchange with the surrounding medium. Our goal is to define the entropy production due to CL propagation in order to identify thermodynamic forces (causes) reciprocal to the rates of translation, rotation, expansion and distortion of the active zone. For this purpose the following assumptions are adopted.

1. Small deformation is considered. The total strain tensor, $\boldsymbol{\epsilon}$, can thus be decomposed into perfectly elastic (thermodynamically reversible) deformation, $\boldsymbol{\epsilon}^{(e)}$; deformation $\boldsymbol{\epsilon}^{(d)}$ resulting from the creation of discontinuities like crazes; and irreversible deformation, $\boldsymbol{\epsilon}^{(i)}$, such as viscous flow:

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{(e)} + \boldsymbol{\epsilon}^{(d)} + \boldsymbol{\epsilon}^{(i)} \quad (2)$$

Accordingly, the total work ($W = \int_V \boldsymbol{\sigma} : \boldsymbol{\epsilon} dv$; where $\boldsymbol{\sigma}$ is the stress tensor, and v is the volume) can be decomposed into three corresponding components:

$$W = W_e + W_d + W_i \quad (3)$$

2. A part, D of the work, W_i , done on irreversible deformation is dissipated on damage formation. The rest of W_i is converted into heat Q . Thus, the rate of energy dissipated on damage formation and growth \dot{D} is defined as

$$\dot{D} = \dot{W}_i - \dot{Q} \quad (4)$$

Since $\dot{\rho} = 0$ everywhere outside of the active zone, \dot{D} is localized only within the active zone. Outside of the active zone, the work done on irreversible deformation is totally converted into heat.

3. The Helmholtz free energy, F , of the solid is presented as the sum

$$F = F_0 + F_e \quad (5)$$

where F_0 is the free energy of the unstressed state and F_e is the elastic strain energy. The first term F_0 becomes significant when discontinuities (cracks, crazes, etc.) are introduced. Equation 5 implies that no Helmholtz free energy is associated with irreversible deformation.

4. Gibbs potential, G , is introduced as

$$G = P_0 + P_e \quad (6)$$

where the elastic potential energy P_e is conventionally described as the difference between the elastic strain energy F_e and the work done on elastic deformation, W_e :

$$P_e = F_e - W_e \quad (7)$$

Similarly, the potential energy of the initial unstressed state, P_0 , is introduced as

$$P_0 = F_0 - W_d \quad (8)$$

The latter reflects the potential energy change due to damage.

5. Crack propagation is analysed under isothermal conditions with zero gradient of temperature. It follows that all heat generated within the system is radiated in an equilibrated fashion.

Based on the above statements, the entropy production due to CL propagation has been derived as [17].

$$T\dot{S}_i = \dot{D} + \dot{l}X^{\text{tr}} + \dot{\omega}X^{\text{rot}} + \dot{e}X^{\text{exp}} + \dot{\mathbf{d}}X^{\text{dev}} \quad (9)$$

where X^{tr} , X^{rot} , X^{exp} and X^{dev} are generalized forces reciprocal to the corresponding fluxes \dot{l} , $\dot{\omega}$, \dot{e} , and $\dot{\mathbf{d}}$. Each of these forces is given by the negative first partial derivative of Gibbs potential, G , with respect to the corresponding generalized coordinate. Thus, for example, the driving force for CL translation, X^{tr} , is given by

$$X^{\text{tr}} = -\frac{\partial G}{\partial l} \quad (10)$$

According to the presentation of Gibbs potential given in Equation 6, the translational force consists of two components. The first is the active part

$$J_1 = -\frac{\partial P_e}{\partial l} \quad (11)$$

which is the conventional energy release rate. The second is the resistant part [17]

$$-\gamma^*R_1 = -\frac{\partial P_0}{\partial l} \quad (12)$$

where γ^* is the specific enthalpy of damage and R_1 is the CL translational resistance moment. Thus, the thermodynamic force results from the competition between the active and the resistant tendencies. Below, we present a brief description of γ^* and R_1 .

3.1. The specific enthalpy of damage

Damage events commonly encountered in polymers, such as crazes and shear bands, are considered as discontinuities and characterized by their middle surfaces. The difference between the enthalpy densities of damaged and initial matter multiplied by the thickness of an element of damage (craze or shear band) represents the specific enthalpy of damage with dimensions of Jm^{-2} . Referring to Figs. 1 and 2, CL propagation is accompanied by damage nucleation and growth. This constitutes an energy sink which is the source of resistance to propagation. Thus, the translational resistance moment R_1 accounts for the total amount of damage increment associated with CL advance, and is given by the following integral over the trailing edge $\Gamma^{(t)}$:

$$R_1 = \int_{\Gamma^{(t)}} \rho n_1 d\Gamma \quad (13)$$

where n_1 is the projection of the unit normal vector on the tangent to the crack trajectory at the crack tip [17]. Obviously, the resistance moment is a vector quantity whose magnitude is a pure number. Thus, γ^*R_1 has the dimension of Jm^{-2} . It is worth noting that the energy release rate J_1 is also a vector quantity with direction along the tangent of the crack trajectory (for smooth trajectories). Since J_1 and γ^*R_1 have the same direction which is uniquely defined for a given crack path, it is convenient to use the same symbols for the magnitude of these vectors. That is, J_1 and γ^*R_1 are used to express $|J_1|$ and $|\gamma^*R_1|$, respectively.

3.2. Translation driving force

From Equation 10, using Equations 6, 11 and 12, translational force is expressed as

$$X^{\text{tr}} = J_1 - \gamma^*R_1 \quad (14)$$

The first term, the energy release rate, expresses the amount of energy available for CL translation. The second, on the other hand, is the amount of energy required for nucleation and growth of the damage surrounding the crack and the crack itself. Thus, the magnitude of the thermodynamic force represents the energetic barrier for CL advance.

Other thermodynamic forces, i.e. X^{rot} , X^{exp} and X^{dev} possess similar structure.

4. Law of translational CL propagation

For the case considered, i.e., CL propagation by translational mode alone, Equation 9 reduces to:

$$T\dot{S}_1 = \dot{D} + \dot{X}^{\text{tr}} \quad (15)$$

Upon substitution of Equation 14 into Equation 15, we obtain:

$$T\dot{S}_1 = \dot{D} + \dot{I}(J_1 - \gamma^*R_1) \quad (16)$$

According to the second law of thermodynamics, the entropy production is non-negative, i.e.,

$$T\dot{S}_1 \geq 0 \quad (17)$$

Analysis of stability shows that $J_1 - \gamma^*R_1$ is non-positive for slow crack propagation [17]. Hence, CL propagation is prohibited by the second law unless the first term, \dot{D} , of Equation 16 provides enough dissipation to compensate for the negative term $\dot{I}(J_1 - \gamma^*R_1)$.

Usually, the constitutive equations relating thermodynamic fluxes and forces are obtained from various formulations of the second law as a variational principle. Applying the principle of minimal entropy production, which yields $\dot{S}_1 = 0$ for this case, we obtain the law of CL propagation from Equation 16 as:

$$\dot{I} = \frac{\dot{D}}{\gamma^*R_1 - J_1} \quad (18)$$

The denominator represents the energetic barrier for CL propagation.

The rate of energy dissipated on damage formation and growth, \dot{D} , can be assumed proportional to the total dissipated work, W_1 . The coefficient of proportionality apparently depends on the mechanism of dissipation. One would expect this coefficient to be dependent on strain rate, temperature and the characteristic time of the fracture process. Previously, \dot{D} was approximated as a linear function of the total potential energy $P_e = -\int_0^l J_1(l)dl$ [7]. On the basis of recent developments in CL stress analysis, W_1 can be approximated by the product $J_1 \langle d \rangle$, where $\langle d \rangle$ stands for a characteristic size of the active zone. Thus, \dot{D} can be expressed by

$$\dot{D} = \beta_1 J_1 \langle d \rangle \quad (19)$$

where β_1 is a phenomenological coefficient with the dimension of sec^{-1} . In principle, \dot{D} can be directly evaluated according to Equation 4 as the

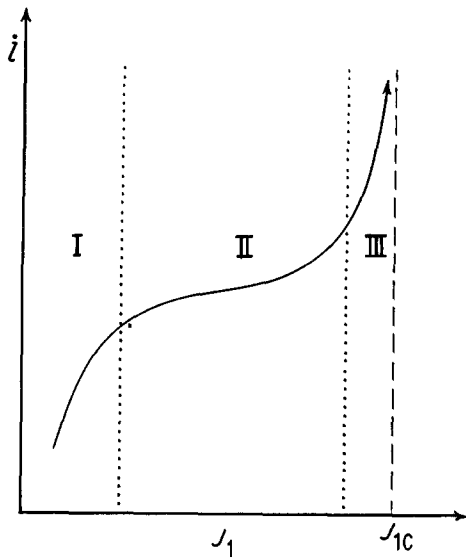


Figure 3 Qualitative crack propagation behaviour according to Equation 20.

difference $\dot{W}_1 - \dot{Q}$. Whereas the total dissipative work \dot{W}_1 is readily measurable from the hysteresis loop, the heat radiated by the active zone \dot{Q} can be measured using, for instance, infrared microscopy.

Substituting Equation 19 into Equation 18, the law of CL translation (propagation) is given by:

$$i = \frac{\beta_1 J_1 \langle d \rangle}{\gamma^* R_1 - J_1} \quad (20)$$

The qualitative behaviour of Equation 20 is expressed in Fig. 3. One can distinguish three stages of slow CL propagation. In stage I, the CL translational resistance moment, R_1 , is very small since the crack propagates through the material damaged during the initiation period. For this reason the initial slope of the \dot{l} versus J_1 curve is relatively high. Stage II, an intermediate stage, is characterized by damage growth accompanying crack propagation. This is reflected as an increase in R_1 yielding a decreasing slope. In these two stages, CL propagation is controlled by the dissipative mechanisms reflected in \dot{D} (numerator in Equation 20). Finally, when J_1 approaches $\gamma^* R_1$, the crack can undergo a transition from slow to uncontrolled (avalanche-like) mode of propagation (stage III). This transition occurs for unstable configurations [8, 18].

5. Applicability to CL propagation data

The law of CL propagation as presented in Equation 20 was applied to recent measurements on

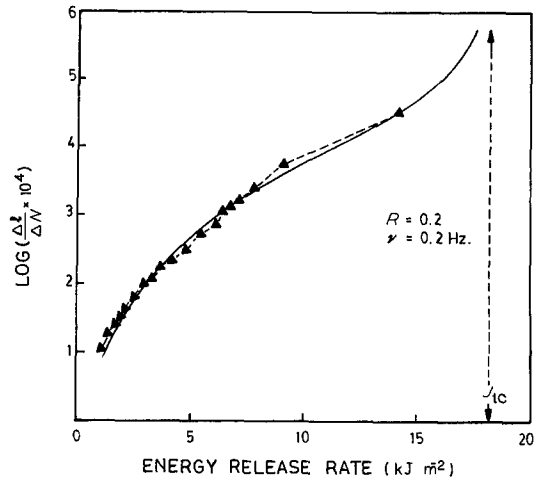


Figure 4 Experimental fatigue crack layer propagation data [11] plotted in terms of Equation 19 (solid line).

polystyrene under cyclic loading conditions (Fig. 4). In this experiment, which is detailed in a forthcoming publication [11], evolution of the CL was measured using time-lapse optical microscopy. From this, the CL length, l , and width, $\mathcal{W}(l)$, were evaluated as a function of the number of cycles. In order to apply Equation 20 to experimental results the following treatment was adopted.

1. The magnitude of the translational resistance moment R_1 can be deduced from Equation 13,

$$R_1 = \int_{\Gamma} \rho n_1 d\Gamma = \int_{-\mathcal{W}/2}^{\mathcal{W}/2} \rho dx_2 = \langle \rho \rangle \mathcal{W} \quad (21)$$

where $\langle \rho \rangle$ expresses damage (crazing) density averaged along the trailing edge of the active zone, and \mathcal{W} is the width of the active zone measured at the crack tip (see Fig. 2). Due to the fact that the CL propagates in a self-similar fashion [11], the average damage density $\langle \rho \rangle$ is considered constant.

2. At critical (avalanche-like) CL propagation, we may write

$$J_{1c} = \gamma^* R_{1c} = \gamma^* \langle \rho \rangle \mathcal{W}_c \quad (22)$$

where the suffix, c, indicates the value of the involved parameter at the critical stage. Accordingly, the term $\gamma^* R_1(l)$ in the denominator of Equation 20 may be expressed by

$$\gamma^* R_1(l) = J_{1c} \frac{\mathcal{W}(l)}{\mathcal{W}_c} \quad (23)$$

3. The characteristic size of the active zone $\langle d \rangle$ is taken as its length l_a (see Fig. 2).

4. In the case considered here, the dissipative coefficient β_1 which has the dimension of sec^{-1} is assumed to be inversely proportional to the life time of the active zone. This is the period of time within which the active zone is "active", i.e., $\rho > 0$ which is the time required by the crack to propagate from the trailing to the leading edge. It has been experimentally determined [11] that this time is inversely proportional to the square of the energy release rate. Therefore, β_1 was calculated from the phenomenological relationship

$$\beta_1 = \beta_0 J^2 \quad (24)$$

For the loading conditions indicated in Fig. 4, β_0 was found to be 4.6×10^{-3} from least square analysis.

From the above analysis, the parameters needed to calculate the rate of CL propagation in terms of the proposed law are J_{1c} , \mathcal{W}_c and $\mathcal{W}(l)$ which are experimentally measured. Only one fitting parameter, i.e., the coefficient β_0 of Equation 24, is employed. Fig. 4 shows the extent of agreement between the data and the proposed formalism within a range of four orders of magnitude of the crack speed.

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