A THEORY FOR TRANSLATIONAL CRACK LAYER PROPAGATION

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ABSTRACT

A theory is presented to model the propagation of a crack preceded by evolving damage. The crack and the surrounding damage are treated 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 translational CL propagation as:

$$\dot{\ell} = \frac{\beta_1 W_i}{\gamma^* R_1 - J_1}$$

where $\dot{\ell}$ is the CL length, β_1 is a dissipative coefficient expressing the fraction of the total irreversible work W_i, expended on CL translation, J_1 is the energy release rate, γ^* is the specific enthalpy of damage and R_1 is the translational resistance moment. This expression describes the entire history of CL propagation. All parameters involved can be experimentally measured except β_1 which is presently taken as a phenomenological coefficient.

KEYWORDS

Damage, Entropy production, Crack Layer, Specific enthalpy of damage, Energy release rate, Translational resistance moment, Crack propagation.

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 co-workers. 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. 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 submicroscopic 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 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.

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 (Kitagawa, 1983). 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" (Bakar, Moet and Chudnovsky, 1983; Haddaoui, Chudnovsky and Moet, 1983). For example, Fig. 1 exhibits layers of extensive damage accompanying fatigue crack propagation in stainless steel (Chudnovsky and Bessendorf, 1983) and polypropylene (Chudnovsky and co-workers, 1983). A similar CL is also displayed by polystyrene as shown in a companion paper (Botsis, Chudnovsky and Moet, 1984a). Although these materials are structurally different, the macroscopic evolution of damage appears strikingly similar. Similar features of fracture propagation have been observed recently in materials as well (Hoagland, Han and Rosenfield, 1974; D. Clark, 1983). A rational model of fracture propagation has to account for the fracture phenomenon as observed.

Two complimentary 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 (Chudnovsky and Kachanov, 1983; Dolgapolsky, 1983) describe early results of elastic crack-damage interaction. The general thermodynamic framework of the crack layer theory is presented by Chudnovsky (1983). In the present paper, the discussion is limited to a thermodynamic treatment of crack layer propagation by translational mode.

DAMAGE DENSITY

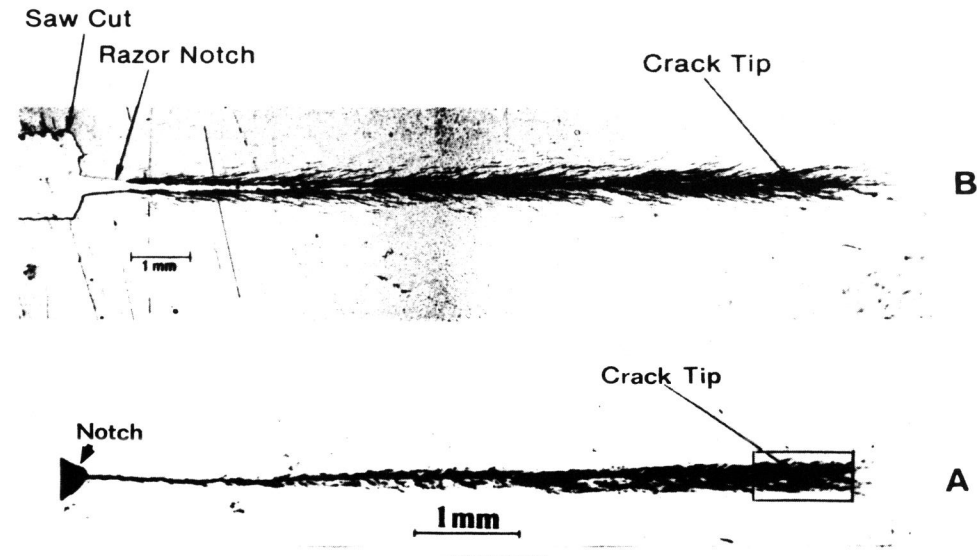In our model, damage is defined as discontinuities such as microcracks,

Fig. 1 Optical micrographs of SEN specimens of stainless steel (A) and polypropylene (B) under fatigue loading. The propagating crack is preceded and surrounded with damage.

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^2/m^3. For example, the craze density in the vicinity of the main crack has been directly evaluated from optical micrographs of thinned polypropylene samples (Chudnovsky and co-workers, 1983). A more complete description of damage requires an additional parameter characterizing orientation. In this paper, since we consider rectilinear crack propagation where no change in damage orientation occurs, ρ suffices for damage characterization.

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 a 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 Tg, the rate of damage change (further growth or healing) under unloading conditions is assumed 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 ($\Gamma^{(\ell)}$) and a trailing edge ($\Gamma^{(t)}$) (Fig. 2). Motion of the active zone, in
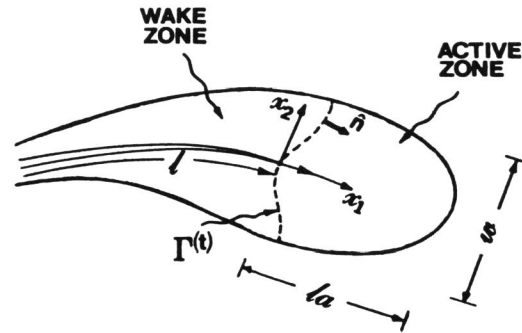
Fig. 2. A schematic illustration of a crack layer in an infinite plane.

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 $\dot{\ell}$, rotation $\dot{\omega}$, isotropic expansion $\dot{e}$, and distortion $\dot{d}$ are considered as thermodynamic fluxes. The law of CL propagation is thus established by relating these fluxes to the reciprocal forces (causes) within the framework of irreversible thermodynamics.

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

$$\dot{S}^{TOT} = \dot{S}_i + \dot{S}_e \tag{1}$$

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.

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

flow, i.e.,

$$\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^{(e)} + \underset{\sim}{\varepsilon}^{(d)} + \underset{\sim}{\varepsilon}^{(i)} \tag{2}$$

Accordingly, the total work ($W = \int_v \underset{\sim}{\sigma} : \underset{\sim}{\varepsilon} \, dv$; where $\underset{\sim}{\sigma}$ is the stress tensor, and v is the volume) can be decomposed into three corresponding components, i.e.,

$$W = W_e + W_d + W_i \tag{3}$$

(ii) 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

$$\dot{D} = \dot{W}_i - \dot{Q} \tag{4}$$

Since $\rho = 0$ 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.

(iii) The Helmholtz free energy, F, of the solid is presented as the sum

$$F = F_o + F_e \tag{5}$$

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

(iv) Gibbs potential, G, is introduced as

$$G = P_o + P_e \tag{6}$$

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), i.e.,

$$P_e = F_e - W_e \tag{7}$$

Similarly, the potential energy of the initial (unstressed state "P_o" is introduced as

$$P_o = F_o - W_d \tag{8}$$

The latter reflects the potential energy change due to damage.

(v) Crack propagation is analyzed under isothermal conditions with zero gradient of temperature. It follows that all heat generated within the system is radiated in equilibrial fashion.

Based on the above statements, the entropy production due to CL propagation has been derived as (Chudnovsky, 1983)

$$T\dot{S}_i = \dot{D} + \dot{\ell} \cdot X^{tr} + \dot{\omega} \cdot X^{rot} + \dot{e} \cdot X^{exp} + \dot{\underset{\sim}{d}} \cdot X^{dev} \tag{9}$$

where X^{tr}, X^{rot}, X^{exp} and X^{dev} are generalized forces reciprocal to the corresponding fluxes $\dot{\ell}$, $\dot{\omega}$, $\dot{e}$, $\dot{d}$. 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

$$X^{tr} = - \frac{\partial G}{\partial \ell} \qquad (10)$$

According to the presentation of Gibbs potential given in (6), the translational force consists of two components. The first is the <u>active</u> part

$$J_1 = - \frac{\partial P_e}{\partial \ell} \qquad (11)$$

which is the conventional energy release rate. The second is the <u>resistant</u> part (Chudnovsky, 1983)

$$\gamma \star R_1 = - \frac{\partial P_o}{\partial \ell} \qquad (12)$$

where $\gamma\star$ is the specific <u>enthalpy of damage</u> and R_1 is the <u>CL translational resistance moment</u>. Thus, the thermodynamic force results from the competition between the active and the resistant tendencies. Below, we present a brief description of $\gamma\star$ and R_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 (microcrack, craze or shear band) represents the <u>specific enthalpy of damage</u> with dimensions of J/m^2. Refering 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 <u>translational resistance moment</u> 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 $\Gamma^{(t)}$

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

where n_1 is the projection of the unit normal vector on the tangent to the crack trajectory at the crack tip. Obviously, the resistance moment is a vector quantity whose magnitude is a pure number. Thus, $\gamma\star R_1$ has the dimension of J/m^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 $\gamma\star R_1$ 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 $\gamma\star R_1$ are used to express $|J_1|$ and $|\gamma\star R_1|$, respectively.

CL TRANSLATIONAL DRIVING FORCE

From (10), using (6), (11) and (12), translational force is expressed as

$$X^{tr} = J_1 - \gamma\star R_1 \qquad (14)$$

The first term, the energy release rate, expresses the amount of energy <u>available</u> for CL translation. The second, on the other hand, is the amount of energy <u>required</u> 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.

LAW OF TRANSLATIONAL CL PROPAGATION

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

$$T\dot{S}_i = \dot{D} + \dot{\ell} \cdot X^{tr} \qquad (15)$$

Upon substitution of equation (14) into (15), we obtain:

$$T\dot{S}_i = \dot{D} + \dot{\ell}(J_1 - \gamma\star R_1) \qquad (16)$$

According to the second law of thermodynamics, the entropy production is non negative and equals zero for reversible processes, i.e.,

$$T\dot{S}_i \geq 0 \qquad (17)$$

Analysis of stability shows that $J_1 - \gamma\star R_1$ is nonpositive for slow crack propagation (Chudnovsky, 1983). Hence, CL propagation is prohibited by the second law (17) <u>UNLESS</u> the first term $(\dot{D})$ of equation (16) provides enough dissipation to compensate for the negative term $\dot{\ell}(J_1 - \gamma\star R_1)$.

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

$$\dot{\ell} = \frac{\dot{D}}{\gamma\star R_1 - J_1} \qquad (18)$$

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_i). 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. On the basis of recent developments in CL stress analysis (Botsis, Chudnovsky and Moet, 1984b) W_i is

xxxxxxx from experimental observations as the work done by the boundary forces on the displacement at the grips due to discontinuities evolved with-

in the active zone. Thus $\dot{D}$ can be expressed by

$$\dot{D} = \beta_1 W_1 \tag{19}$$

where β_1 is the phenomenological coefficient with the dimension of sec^{-1}. In principle, $\dot{D}$ can be directly evaluated according to equation (4) as the difference $W_1 - \dot{Q}$. Whereas the total dissipative work W_1 is readily measurable from the hysteresis loop, the heat radiated by the active zone Q can be measured using, for instance, infrared microscopy.

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

$$\dot{\ell} = \frac{\beta_1 W_1}{\gamma^* R_1 - J_1} \tag{20}$$

The qualitative behavior of equation (20) is expressed in Fig. 3. One can distinguish three stages of slow CL propagation. In stage I, the CL transla-tional resistance moment (R_1) is very small since the crack propagates through

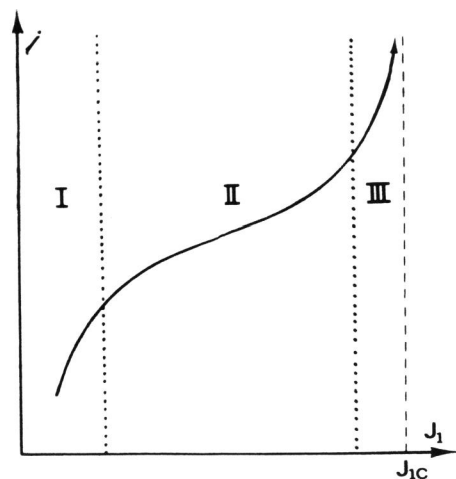Fig. 3. Qualitative crack propagation behavior according to equation (20).

the material damaged during the initiation period. For this reason the ini-tial slope of $\dot{\ell}$ vs. 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 20). Finally, when J_1 approaches $\gamma^* R_1$, the crack can un-dergo a transition from slow-to-uncontrolled (avalanche-like) mode of propa-gation (stage III). This transition occurs for unstable configurations (Sehanobish and co-workers, 1984).

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