

ENERGY EQUILIBRIA AND RATE PROCESS
IN BRITTLE FRACTURE

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So as to treat brittle fracture by an atomic model, problems in the energy equilibria on the crack stability and those in the rate process are discussed, and new expressions are proposed. Newly derived critical condition of crack propagation for Griffith type through microcrack in brittle material is given as follows,

$$\sigma_0 = 2(E\gamma_s/l)^{1/2}$$

where, σ_0 ; critical tensile stress (threshold stress of subcritical crack growth) operated normal to crack surface and parallel to specimen length, E ; Young's modulus, γ_s ; surface free energy of the material, l ; specimen length.

And it is shown that the following formulation of rate equation is useful to explain the velocity of crack propagation.

$$v = f\{\exp(-\Delta G_a/RT)\} \cdot \psi \cdot \{1 - \exp(-\Delta G_0/RT)\}$$

Where, v ; velocity of the reaction like crack propagation, f ; frequency factor, ΔG_a ; activation energy necessary for the reaction remarked, ψ ; measure unit of the reaction rate (in case of crack propagation, i.e. a lattice parameter), ΔG_0 ; excess free energy stored in the system which is expected to be finally dissipated through the reaction.

The term expressed in the parenthesis, { } corresponds to an effective probability of the transformation and it becomes zero under the critical (i.e. equilibrium) condition. A pair of these equations makes it possible to treat the equilibrium and the rate process continuously.

PREFACE

Stability of a crack in brittle materials under load is a problem of thermodynamic equilibrium and the velocity of crack propagation is a problem of reaction rate. In the present report, both problems are discussed basically.

STABILITY OF CRACK

According to thermodynamics, an equilibrium of two different states of same material is expressed by the equality of their free energy level. Consider the two different states as shown in Fig. 1. If the crack size $2C$ satisfies a condition $2C \ll t < w \sim 1$, and the product, $(l \cdot t \cdot w)$ is equal to molar volume V , choosing stress free and crack free state of same size of material as the reference state, the free energy level of the state I can be well approximated by following equation,

$$\Delta G_I = (\sigma^2 V / 2E) \quad (1)$$

where the σ is uniform tensile stress operated at the boundary normal to the crack surface and along the direction of l .

Since the state F is free from stress and free from kinetic energy, the excess free energy stored in the system is only the surface free energy necessary to separate the specimen in two pieces. That is,

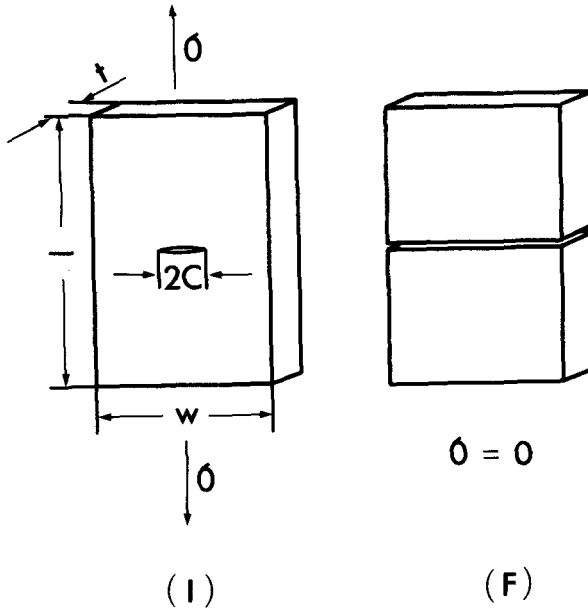


Fig. 1

Defined initial state (I) and final state free from kinetic energy (F).

$$\Delta G_F = 2\gamma_s tw = (2V\gamma_s/l) \quad (2)$$

The thermal equilibrium between state I and F is given by a condition, $\Delta G_I = \Delta G_F$, and following relation is obtained [1].

$$\sigma_0 = 2(E\gamma_s/l)^{1/2} \quad (3)$$

Where, σ_0 is the critical stress of crack extension, i.e. the threshold stress of subcritical crack growth. If additional works are concerned with γ_s , one can add those works to the γ_s .

Though, similar condition to Eq. (3) is already discussed by Griffith [2,3], in case of his system, the same treatment with Eq. (1) - (3) gives a result, $\sigma_0 = 0$. Since his system is characterized by infinite value of l and w .

RATE EQUATION TO EXPRESS REACTION OCCURRED IN HETEROGENEOUS SYSTEMS

There have been proposed many experimental and theoretical formulae [4-7], but all of these proposals have not succeeded to take into account the threshold condition of the crack propagation. This problems can be solved by application of a new proposal for the generalized expression of the rate process [8]. That is,

$$v = f \{ \exp(-\Delta G_a / RT) \} \cdot \psi \cdot \{ 1 - \exp(-\Delta G_0 / RT) \} \quad (4)$$

Where, v ; velocity of the reaction, f ; frequency factor, ΔG_a ; activation energy of a reaction remarked, ψ ; measure unit of the reaction rate (in case of crack propagation, i.e. lattice parameter), ΔG_0 ; excess energy stored in the system which is finally dissipated through the reaction (in case of crack propagation, i.e. the energy difference, $\Delta G_I - \Delta G_F$ in Fig. 1), R ; gas constant, and T ; absolute temperature.

The term expressed in the parenthesis, $\{ \}$ corresponds to an effective probability of transformation of the reaction and it becoms zero under the equilibrium state expressed in the former section. The expression of Eq. (4) is useful to treat a rate process occurred in heterogeneous system such as crack propagation, and it makes possible to treat the equilibrium and the rate process continuously. Similar expressions to Eq. (4) have successfully applied for the explanation of diffusion controlled mass transport in heterogeneous systems [9].

RATE OF CRACK PROPAGATION

Consider a system illustrated in Fig. (1)-I, and assume $2C$ and the stress satisfying $2C \ll t < w \sim 1$ and $\sigma > \sigma_0$. Under the condition, the details of Eq. (4) can be shown as follows,

$$v = (n'/n)(RT/Nh) \left[\exp\{(\Delta G_{\sigma_m} - \Delta G_{th})/RT\} \right] \cdot \lambda \cdot \{1 - \exp(-\Delta G_0/RT)\} \quad (5)$$

where, n ; number of atomic pairs which must be broken to advance crack an atomic spacing, n' ; number of atomic pairs bearing maximum stress at the crack tip, N ; Avogadro's number, h ; Planck's constant, ΔG_{σ_m} ; molar strain energy stored in the atomic pair bearing the maximum stress at the crack tip [10], ΔG_{th} ; molar strain energy supposed to be stored in the atomic pair under maximum theoretical stress [11], λ ; lattice spacing along the direction of crack propagation, and ΔG_0 ; excess free energy stored in the system (in case of the example shown in Fig. 1, i.e. $\Delta G_I - \Delta G_F$). In general, $n = n'$ may be preserved.

The ΔG_{th} increases by the introduction of additional works such as dislocation formation and by crack branching, but ΔG_{σ_m} decreases by these processes and by crack blunting. Chemical reactions at the crack tip such as moisture effect, generally decrease ΔG_{th} .

LIFE PREDICTION

The life prediction of precracked specimen by K_I mode becomes possible by the following formula, using Eq. (5),

$$\Delta t = \int_{2C}^w dC/v(C, \sigma) \quad (6)$$

and if ΔG_{σ_m} is linearly proportional to the crack length [10], under a condition $w > 20C$, the result of integration of Eq. (6) is given as follows, assuming $n = n'$,

$$\Delta t = \{ \exp(-\Delta G_C/RT) \} / (\Delta G_{\sigma_m}/RTC) (RT/Nh) \lambda (\Delta G_0/RT) \exp(-\Delta G_{th}/RT) \quad (7)$$

where, Δt ; time to failure from crack length C to a catastrophe, ΔG_C ; molar strain energy stored in the atomic pair bearing maximum stress at a crack tip of a crack in length $2C$.

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