THEORETICAL CALCULATION OF THE RATE OF CRACK PROPAGATION AND TIME TO FAILURE IN SiC SINGLE CRYSTAL

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Using new proposals regarding the stability condition of cracks in a brittle material and the rate equations for heterogeneous system, numerical calculations are performed on the rate of crack propagation and the time to failure in silicon carbide single crystal, assuming Griffith type atomically sharp crack and linear elasticity in the material.

A technological expression of K_I - v relation is proposed as follows,

$$v = A \left[\exp\{(B\ K_I^2 - C)/RT\} \right] \cdot (K_I^2/C)$$

where, v; verocity of crack propagation, C; half length of Griffith type crack, K_I; stress intensity factor near by the crack tip, R; gas constant, T; absolute temperature, and A, B and C are material constants.

PREFACE

In the present report, the rate of crack propagation is calculated on silicon carbide single crystal, using a new proposal to treat the rate process in heterogeneous system [1]. The basic equation is,

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

where, v; velocity of crack propagation, n; number of atomic pairs which must be separated to advance crack an atomic spacing, n'; number of atomic

pairs bearing maximum stress at the crack tip, N; Avogadoro's number, h;

Planck's constant, $\Delta G_{\sigma m}$; molar strain energy stored in the atomic pair

bearing the maximum stress at the crack tip [2], ΔG_{th}; molar strain energy

supposed to be stored in the atomic pair under maximum theoretical stress

[3], λ; lattice spacing along the direction of the crack propagation, and

ΔG_0; excess free energy stored in the system which is expected to be

finally relaxed through the separation of material in two pieces (in case

of Griffith type microcrack, that is the strain energy finally turning

into kinetic energy by the separation).

ASSUMPTIONS AND NUMERICAL DATA USED IN THE CALCULATION

Linear elasticity is assumed, and the atomic force between adjacent

atoms is supposed to be expressed as follows,

$$\text{if } a_0 \leq a \leq a_{th}; \qquad \sigma = E(a - a_0)/a_0$$
$$\text{and if } a > a_{th}; \qquad \sigma = 0 \tag{2}$$

where, a_0; atomic distance between atoms under stress free state, a; the

distance under stress σ, a_{th}; the distance under maximum theoretical

stress.   The maximum theoretical stress, σ_{th} which corresponds to a_{th},

is supposed to follow Orowan's expression [3],

$$\sigma_{th} = (E\gamma_s/a_0)^{1/2} \tag{3}$$

where, E; Young's modulus.

The maximum stress realized in the specimen which has a Griffith type

atomically sharp crack, is assumed to be expressed by the result of Inglis

[2]. Assuming the radius of curvature at the crack tip being $a_0/2$, and

using V for molar volume, the stress σ_m is,

$$\sigma_m = (8C\sigma^2/a_0)^{1/2} \tag{4}$$

From Eq. (2)-(4), assuming a Griffith type microcrack in the specimen, ΔG_{th}, $\Delta G_{\sigma m}$ and ΔG_0 in Eq. (1) are given as follows,

$$\Delta G_{th} = (E\gamma_s/a_0)(V/2E) \tag{5}$$

$$\Delta G_{\sigma m} = (8C\sigma^2/a_0)(V/2E) \tag{6}$$

$$\Delta G_0 = (\sigma^2 V/2E) - (2V\gamma_s/l) \tag{7}$$

Physical data used in the next section for an actual calculation of the rate of crack propagation in (111) plane of β-SiC are, V; 1.261×10^{-5} m^3/mol, γ_s; 3.17 J/m^2, a_0; 2.518×10^{-10} m, and E; 4.6×10^{11} Pa.

RATE EQUATION AND EQUATION FOR THE TIME TO FAILURE

Since $n = n'$ may be realized for the Griffith type through crack, Eq. (1) can be rewritten, using Eq. (5)-(7),

$$v = (dC/dt) = (RT/Nh)\left[\exp\{(V/2ERTa_0)(8C\sigma^2 - E\gamma_s)\}\right]\cdot\lambda\cdot$$
$$\cdot\left[1 - \exp(1/RT)\{(2V\gamma_s/l) - (\sigma^2 V/2E)\}\right] \tag{8}$$

and under the condition, $\Delta G_0 \ll RT$ and $(\sigma^2 V/2E) \gg (2V\gamma_s/l)$, following equation gives an apploximation to Eq. (8).

$$v = (RT/Nh)\left[\exp\{(V/2ERTa_0)(8C\sigma^2 - E\gamma_s)\}\right]\cdot\lambda\cdot(\sigma^2 V/2ERT) \tag{9}$$

The result of calculation of Eq. (9) at 293 °K is shown in Fig. 1. If one takes into account a nonlinear elastic model for the estimation of ΔG_{th} and $\Delta G_{\sigma m}$, v may become smaller than that given by Eq. (9).

Since the time necessary for the crack propagation from crack length C_1 to C_2 is given by the following expression,
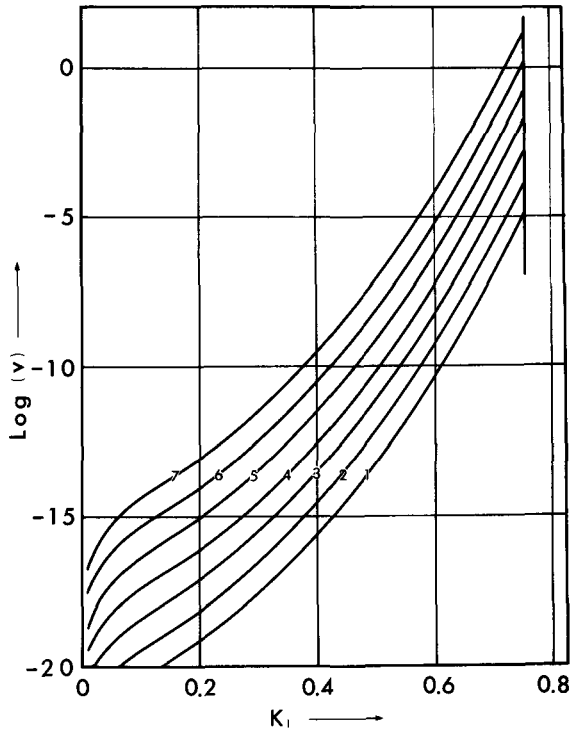
$$\Delta t = \int_{C_1}^{C_2} dC/v(C,\sigma) \tag{10}$$

Fig. 1

Calculated $C(m)-K_I(MN/m^{3/2})-v(m/sec)$ relation at 293 °K in (111) plane of β-SiC single crystal by Eq. (9). The number attached to each curve corresponds to the power n in the relation $C = 10^{-n}$ (m).

where, C_1; half length of the initial crack, C_2; half length of the crack after the propagation by a stress σ for a period, Δt.

Integration of Eq. (10) using Eq. (9) for v(C,σ) leads to the folowing results.

$$\Delta t = \frac{\left[\exp(-8C_1\sigma^2V/2ERTa_0)\right] - \left[\exp(-8C_2\sigma^2V/2ERTa_0)\right]}{(8\sigma^2V/2ERTa_0)(RT/Nh)\cdot\lambda\cdot(\sigma^2V/2ERT)\ \exp(-VE\gamma_s/2ERTa_0)} \tag{11}$$
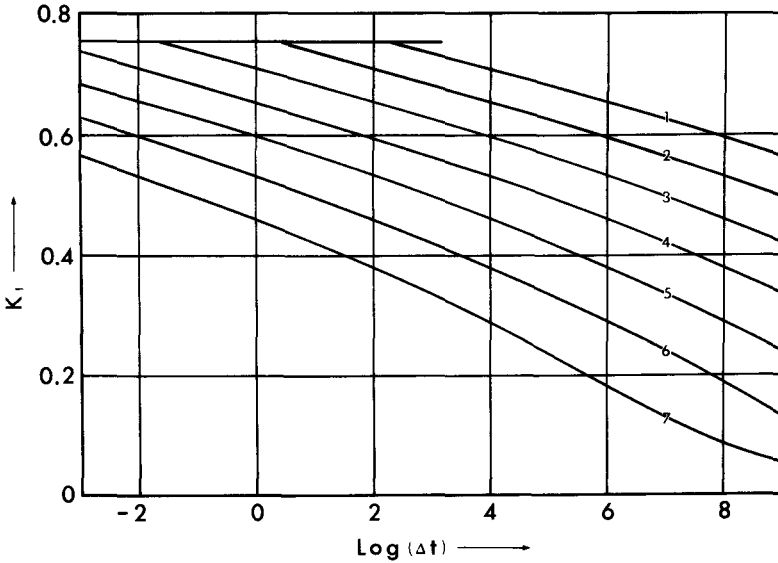
Fig. 2

Calculated C(m)-K_I(MN/m$^{3/2}$)-Δt(sec) relation at 293 °K in (111) plane of β-SiC single crystal by Eq. (11), assuming $C_2 > 10\ C_1$. The number attached to each curve has the same meaning with that in Fig. 1.

The second term of the numerator in the Eq. (11) can be neglected, if $C_2 > 10 C_1$ is preserved. Figure 2 is a result of actual calculation performed under the same condition with Fig. 1. In the calculation, T is choosen at 293 °K and $C_2 > 10\ C_1$ is assumed.

TECHNOLOGICAL EXPRESSION OF K_I - v RELATIONS

The Eq. (8) and (9) leads to a technological expression of K_I - v relations as follows, using a definition, $K_I = \sigma(\pi C)^{1/2}$,

$$v = A \left[\exp\{(B\ K_I^2 - C)/RT\}\right] \cdot (K_I^2/C) \tag{12}$$

where, K_I; stress intensity factor near by the crack tip, **A**, **B** and **C** are material constants, and **B** and **C** are affected by the atomosphere especially in the region of subcritical crack growth [4]. If K_{IC} is concerned with certain velocity of crack propagation, Eq. (12) predicts that the K_{IC} may be affected by crack length.

REFERENCES

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