Oscillatory instability in thermal cracking: A first-order phase-transition phenomenon

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The transition between straight and oscillatory crack propagation is analyzed by simulation of the phenomenon by means of the finite element method. The amplitude of a given undulating crack was found to either increase or decrease in propagation depending on the velocity of the cooling front and the temperature difference. The morphological phase diagram and wavelength obtained in this way are compared with the results of linear stability analyses and experimental data in literature. The postcritical behavior is characterized by a jumplike loss of stability analogous to first-order phase transitions.

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I. INTRODUCTION

Crack pattern formation can be analyzed analogous to other phenomena governed by moving boundary problems, as there are diffusion limited aggregation, dielectric breakdown, and directional solidification, by means of well-known techniques from the theory of nonlinear phenomena. For instance, multiple crack propagation caused by thermal shock was analyzed in [1] by rigorous fracture mechanics and bifurcation theory applied to straight cracks. In this way it became possible to numerically reproduce the experimentally observed hierarchical crack propagation, except for the more or less distinct undulations (Fig. 1 in [1]).

Yuse and Sano [2] carried out an ingeniously simple experiment involving the unusual combination of thermal shock and stationarity, which makes it well suited for the study of thermal shock crack propagation. Their experiment consisted in lowering a hot glass slab with constant velocity v of a few mm/s into cold water, where ΔT was chosen as 50 K to 300 K (Fig. 1). By variation of parameters they found the experimental conditions for the formation of straight or undulating cracks. They represented their results as a morphological phase diagram in the $(v, \Delta T)$ plane.

The experiment was simulated in [3] and [4] by spring models, with the results that there were several morphological phases. However, no quantitative comparison with the experiment was possible. Concerning the wavelengths, theory agreed with experiment.

The boundaries between the morphological phases were calculated by Marder [5] and more appropriately by Sasa, Sekimoto, and Nakanishi [6] by means of fracture mechanics and linear stability analysis. Without considering nonlinear terms, the authors [6] stated that the transition was a Hopf bifurcation. The wavelength turned out too short compared with the experiment [2].

The subjects of this paper are (a) the finite element method (FEM) simulation of experiment, (b) investigation of the transition from straight to undulating cracks, (c) nonlinear analysis of the postcritical behavior with respect to the character of the morphological phase transition (first or second order).

II. CRACK PROPAGATION EQUATION AND FEM TECHNIQUE

We consider a crack propagating stably (i.e., in fracture mechanical equilibrium) as the temperature field is moving along the sample being sunk into the bath. Position and direction of the propagating crack tip are governed by the crack propagation criterion consisting of conditions for the stress intensity factors K_{I} and K_{II}

$$K_{\mathrm{I}} = K_{\mathrm{Ic}}, \quad K_{\mathrm{II}} = 0 . \tag{1}$$

K_{Ic} is a property of the material. The stress intensity factors K_{I} and K_{II} describe the singular stress field σ near the crack tip with respect to opening and shear mode

$$\sigma = \frac{1}{\sqrt{2\pi r}} [K_{\mathrm{I}} f_{\mathrm{I}}(\theta) + K_{\mathrm{II}} f_{\mathrm{II}}(\theta)] . \tag{2}$$

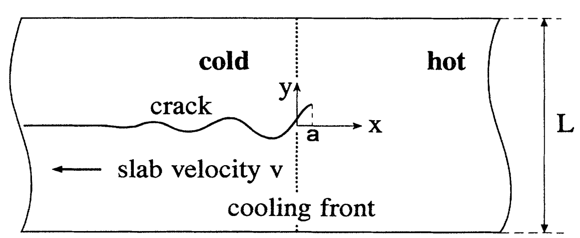

FIG. 1. Scheme of the experiment by Yuse and Sano [2]. The crack tip keeps ahead of the cooling front.

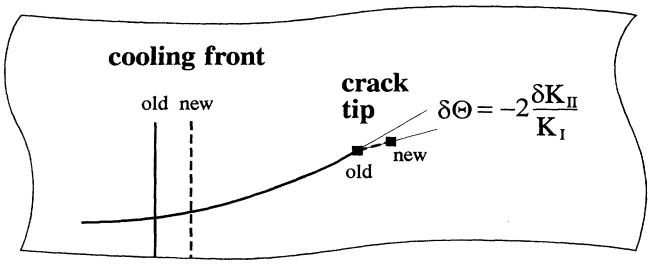

FIG. 2. Incremental step in numerical simulation of crack propagation.

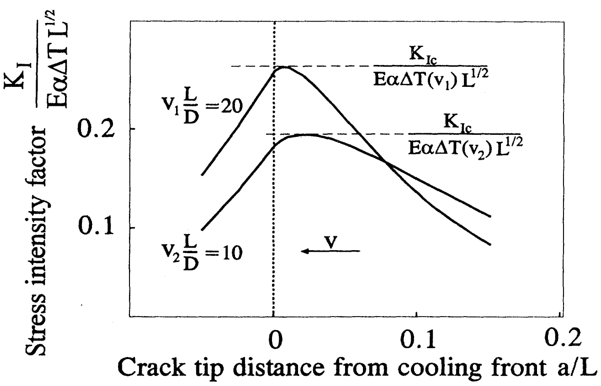

FIG. 3. Normalized stress intensity factor of straight crack vs crack tip distance from cooling front, with velocity as a parameter of the family of curves. Higher ΔT makes a lower position of the K_{Ic} level in this representation. Stationary crack propagation becomes possible if the K_I curve of a given velocity reaches K_{Ic}. This condition is met with a certain $\Delta T(v)$ making up the lower solid curve in Fig. 4.

(σ, $f_{\rm I}$, $f_{\rm II}$ are tensors. r and θ are polar coordinates with respect to the crack tip. A more detailed explanation of the relevance of fracture mechanics for the present problem is given in [6].)

The numerical calculation is carried out in such a way that the cooling front is made to advance incrementally while the crack tip stays put. This makes an incremental violation of (1), which is removed by an incremental adjustment of the crack tip position and direction (Fig. 2). The direction of the increment is given by

$$\delta\theta = -2\delta K_{\rm II}/K_{\rm I} \ . \qquad (3)$$

This relation can be derived from Eq. (31) in [7] for $K_{\rm II}=0$. $K_{\rm I}$ and $K_{\rm II}$ were obtained by solving the thermoelastic problem for plane stress by means of the FEM code MARC [8]. For boundary conditions we chose stress-free crack face and no disturbance of the heat flow by the crack as in [5] and [6]. The coordinate system is chosen such that the bath level is always at $x=0$. The stationary temperature field of the thin strip is given then by the simple solution

$$T(x,v) = \Delta T[1-\exp(-vx/D)] \quad \text{for } x>0 \ . \qquad (4)$$

D is the thermal diffusivity.

The inhomogeneous stress field and the undulating crack shape require some adaption of the FEM grid. By means of a transformation $(x,y)\rightarrow(x',y')$, an initial grid with straight crack is transformed such as to be adapted to the curved crack. The essential properties of the initial grid (boundary conditions, small mesh size near cooling front and crack tip, special crack tip elements) are conserved in the transformation. In order to avoid large deformations of the mesh, the calculations are restricted to small amplitudes.

III. MORPHOLOGICAL TRANSITIONS

For reasons of dimensionality, $K_{\rm I}$ takes the shape

$$K_{\rm I}(a,v) = E\alpha\Delta T\sqrt{L}\, f\left[\frac{a}{L}, \frac{vL}{D}\right] , \qquad (5)$$

for a straight crack where E = Young's modulus, α = thermal expansion coefficient, L = sample width, a = crack tip distance from cooling front. The dimensionless function f is shown in Fig. 3 for two arbitrarily chosen values of vL/D. Since the stresses vanish at large distances, $K_{\rm I}$ approaches zero for $a\rightarrow\pm\infty$. It has a maximum near the cooling front. For crack propagation it is necessary that the $K_{\rm I}(a)$ curve reaches or surpasses $K_{\rm Ic}$. As seen from Fig. 3, the condition of $K_{\rm Ic}$ coinciding with the maximum of the $K_{\rm I}(a)$ curve makes a curve in the $(\Delta T, v)$ plane which has the meaning of a phase boundary in parameter space (lower solid curve in Fig. 4). In order to find the parameter region of undulating cracks, and to make sure that the result does not depend on the arbitrarily chosen initial conditions, we started from a straight crack with a slight kink and from a sinusoidal crack of small amplitude, and calculated the propagation by successive incremental steps according to (1) and (3). We obtained an oscillating crack with growing or decaying amplitude as seen in Fig. 5, depending on ΔT and v. The transition between growth and decay of the amplitude defines another curve in the $(\Delta T, v)$ plane. This curve was assumed to represent the phase boundary between straight and undulating cracks (upper solid curve in Fig. 4).

Comparison with the experiment based on the parameters given in [2] and [6] shows that these results agree tolerably well except for very low velocity. The deviation at low velocity could be due to heat loss of the sample between oven and bath. The deviations of the results in [6] (dashed lines in Fig. 4) might be due to the infinite plate approximation applied there, as already suspected by those authors.

It is seen in Fig. 5 that also in the case of growing amplitude the initial inclination is reduced during the next incremental steps. This seems to prove that a reduction of an initial directional deviation must not be taken as a stability criterion as done in [5].

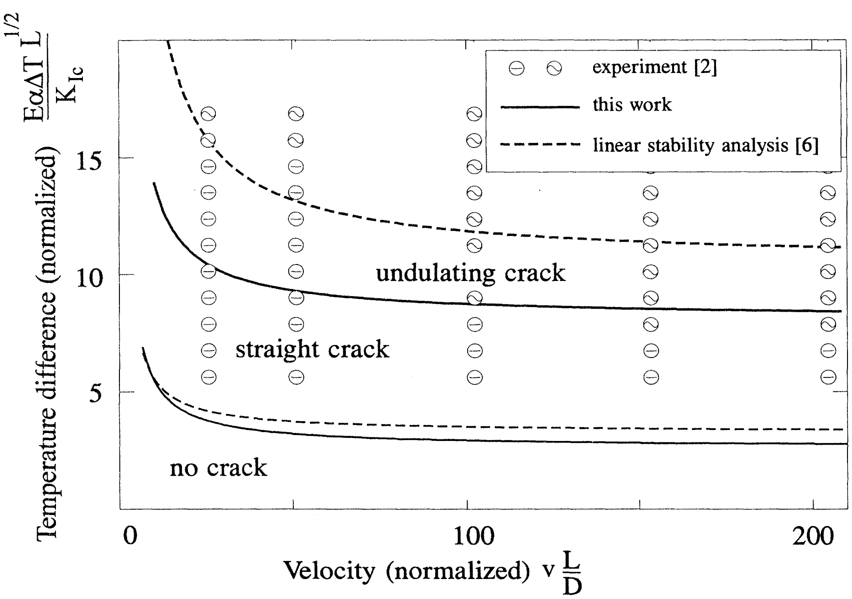

FIG. 4. Morphological phase diagram in normalized $(\Delta T, v)$ space: "no crack/straight crack" boundary, calculated as indicated in Fig. 3, "straight/undulating" boundary, calculated as indicated in Fig. 5, experimental dots after [2].

IV. POSTCRITICAL BEHAVIOR

As an essential advantage of this FEM approach, the type of phase transition can be determined by a nonlinear analysis of the postcritical behavior. The amplitude function or envelope $A(x)$ is assumed to obey an equation

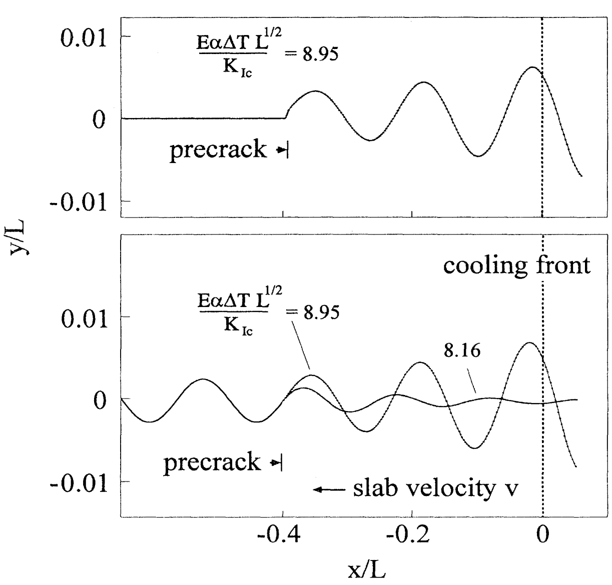

FIG. 5. FEM simulation of oscillatory crack propagation starting from a straight crack with kink and from a sinusoidal crack for $vL/D = 200$. The (small) amplitude decays or increases in propagation depending on ΔT. The transition defines a $\Delta T(v)$ curve representing a phase boundary in parameter space: upper solid curve in Fig. 4. Note that the wavelength appearing in simulated propagation does not depend on the precrack.

$$\frac{dA}{dx} = c_1 \frac{\Delta T - \Delta T_c}{\Delta T_c} \frac{A}{L} + c_3 \left[\frac{A}{L} \right]^3 + c_5 \left[\frac{A}{L} \right]^5 + \cdots , \tag{6}$$

which is an extension of the Ginzburg-Landau equation applied in [2]. Here, even powers of A/L are absent because A and $-A$ should be solutions of this equation. Near ΔT_c, $A(x)$ varies slowly such that the decay or magnification length $l = A/(dA/dx)$ is well approximated by $\lambda A/[A(x+\lambda) - A(x)]$.

L/l as obtained by numerical calculation shows a linear dependence on ΔT and A^2 in good approximation (Fig. 6). The most important information derived from Fig. 6 is $C_3 > 0$. With the assumption of $C_5 < 0$ one obtains the locus of stationary solutions of (6), i.e., $dA/dx = 0$, as in the plot of Fig. 7. So we have not got a supercritical Hopf bifurcation, as suggested in [2], but a subcritical one [9]. Therefore the postcritical behavior is governed by a jumplike loss of stability analogous to a first-order phase transition.

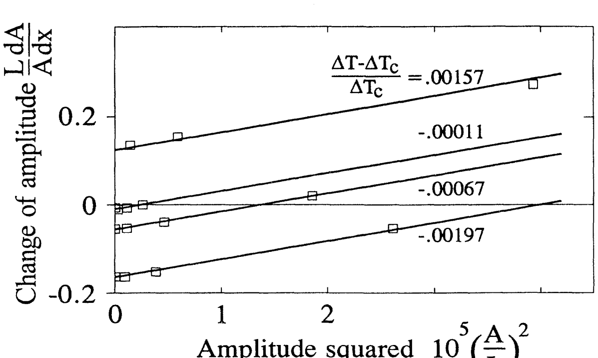

FIG. 6. Characterizing the oscillatory instability as a subcritical Hopf bifurcation: slope implies $C_3 > 0$ in (6). $vL/D = 200$.

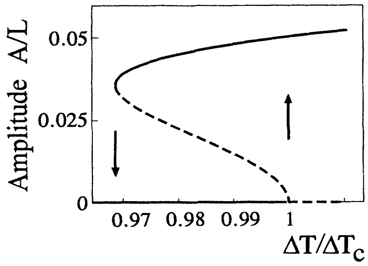

FIG. 7. Stationary solutions of (6) with C_1 and C_3 from Fig. 6 and C_5 from experiment [2]. Solid lines: stable branches; dashed lines: unstable branches. The jumplike loss of stability as indicated by arrows implies hysteresis. Finite fluctuations may give rise to oscillatory propagation also for $\Delta T < \Delta T_c$.

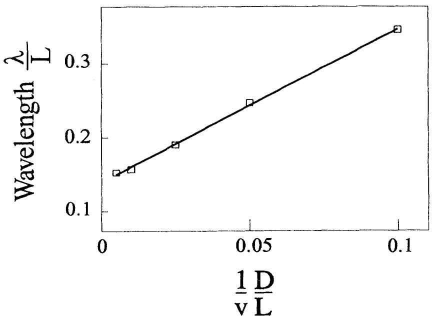

FIG. 8. Wavelength λ/L of simulated cracks on the morphological phase boundary in Fig. 4.

This implies hysteresis, which should show up in experiment. The width of the hysteresis loop in Fig. 7 is given by $\Delta = C_3^2/4C_1|C_5|$, according to (6). From Fig. 6 one obtains $C_1 = 82$ and $C_3 = 4100$. C_5 has been derived from experiment: $A/L \approx 0.05$ for the stationary amplitude near ΔT_c in Fig. 4(a) in [2], combined with the relation $C_3/C_5 = -(A/L)^2$ from (6) for $\Delta T = \Delta T_c$, yields $C_3/C_5 \approx -0.0025$. Hence, $\Delta \approx 0.03$. This makes a rather narrow loop, as seen in Fig. 7. It should be accessible to experimental verification by observing l of nonstationarily oscillating crack propagation. Apparently the data in [2, Fig. 5(a)] were not taken for this purpose and do not happen to cover the parameter region of the hysteresis loop.

Concerning the wavelength, the following can be stated. Since these numerical results are restricted to small amplitudes and therefore are far away from the stationary solution, one cannot expect that the right wavelength comes out. Nevertheless, the calculated wavelength in Fig. 8 seems to be a meaningful quantity as it does not depend on the shape of the arbitrarily chosen initial crack as seen in Fig. 5, and not much on the amplitude. We obtained $\lambda/L \approx 0.14$ for small D/vL, to be compared with 0.05 in [6] and the experimental value 0.28 reported in [2, Fig. 5(b)] (without information on v or ΔT).

Note added in proof. The calculated transition line between straight and undulating cracks in Fig. 4 has been reproduced by the boundary element method. The obtained first-order phase transition may be restricted to large velocities.

V. CONCLUSIONS

We can state that the results of FEM simulation of oscillatory thermal shock crack propagation are similar to the morphological phase diagram and wavelength observed experimentally. A more thorough comparison between numerical simulation and experiment is precluded, at present, by the scarcity of data available in literature. Nonlinear analysis reveals the existence of a jumplike loss of stability analogous to first-order phase transitions. These calculations confirm the result in [6] that the feedback on propagation via change of the temperature field due to the curved crack is not responsible for the oscillation. Its influence on crack propagation is to be investigated by further FEM calculations.

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