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Numerical study of oscillatory crack propagation through a two-dimensional crystal

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We study fracture propagation through a two-dimensional crystal induced by thermal stress by using numerical simulations of a deterministic spring model. Controlling the applied thermal stress, we find several remarkable phases of crack patterns including straight, oscillatory, and branching morphology. We also determine the wavelength of the oscillating cracks at the transition points in accord with experiments by Yuse and Sano [Nature (London) **362**, 329 (1993)].

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The study of crack propagation would have two different major goals. One is for fast crack formation whose time scale is comparable to atomic vibrations and the other is for slow or equilibrium cracks. Equilibrium crack propagation has been studied intensively in engineering fields of science, especially to design desirable constructions of materials. It has also received attention as a problem of physics of pattern formation in complex systems [1–3].

Recently Yuse and Sano [4] reported well-controlled experiments on the equilibrium crack formation of glass plates by applying thermal stress. They prepared very thin glass plates and heated them up first. When the plate was dipped into cool water, they found a variety of propagating crack patterns with good reproducibility. One of the most surprising and nontrivial results of their experiment was the transition from straight cracks to oscillatory ones with a certain wavelength, which could be regarded as a Hopf bifurcation. But the origin of the instability of crack growth and the mechanism of the crack pattern selection still has not been understood well [5–7]. In this Rapid Communication we study a simple spring network model to represent the elasticity of a thermally stressed solid, being inspired by their experiments.

Let us consider, first, elastic properties of a two-dimensional simple square crystal with nearest-neighbor and next-nearest-neighbor interactions. The force between the "atoms" in the crystal is assumed to be proportional to the displacement from the neutral distance, which is represented by Hookean springs with a spring constant, where the springs can be freely rotated around the atoms [8–11]. For simplicity we do not take into account the acoustic vibrations in the crystal at all, thus the mass of the atoms was considered to be exactly zero. Let k_1 be the spring constant for nearest-neighbor interaction and k_2 for next nearest-neighbor interaction, where k_1 and k_2 are related to the coefficients of elastic tensor C_{ijkl} for the two-dimensional crystal on the x-y plane [12]. Then one can easily obtain

$$C_{xxxx}=C_{yyyy}=k_1+k_2 , \tag{1}$$

$$C_{xxyy}=C_{yyxx}=C_{xyyx}=C_{yxxy}=C_{xyxy}=C_{yxyx}=k_2 , \tag{2}$$

and the other coefficients are zero. Note that the lattice constant of the spring network does not affect the elastic characteristics in the two-dimensional system.

Thermal stress is applied to the crystal in the following way as in the experiments we mentioned: Assuming the steady-state thermal diffusion, the temperature T at each spring is given by the following sigmoidal function of vertical position y and time t:

$$T(y,t)=-\frac{\Delta T}{2}\tanh\{\beta[y-y_0(t)]\} , \tag{3}$$

$$y_0(t)=Vt , \tag{4}$$

where ΔT is the temperature difference applied between the top and the bottom of the specimen, V the "dipping" velocity of it into liquid. Here β is a constant comparable to the inverse of the thermal diffusion length $\simeq D/V$ (D is the thermal diffusion constant). In numerical simulations, we simplify Eq. (4) as $y_0=\delta y\, n$, where n is the number of iterative steps corresponding to time and δy a small number (typically one-tenth of the length of springs). Although this T may not be the exact solution of the temperature distribution in the experiment by Yuse and Sano [4], one can expect that the details of T are irrelevant to the results as long as T has an exponential-like decay with the same thermal diffusion length. Next, we assume the natural distances of the springs to be a linear function of local temperature. According to the temperature, the equilibrium length $a_0(y)$ of springs is determined as

$$a_0(y,n)=a_0[1+\alpha T(y,n)] , \tag{5}$$

where a_0 is the lattice constant of the stress-free crystal and α the thermal expansion coefficient. Since the springs have a length, temperature is evaluated at the middle point of each spring. Now we can calculate the equilibrium configuration of the spring network making use of a simple relaxation method. In our simulations, relative error of the equilibrium position of nodes was smaller than 10^{-5}.

Here we introduce a deterministic rule for breaking springs (bonds), rather than stochastic rules [9,11], according to the applied thermal stress. When the force given on a spring exceeds a critical value, it breaks, i.e.,

the corresponding spring constant changes to be zero from k_1 or k_2, which can be regarded as a microscopic interpretation of the failure criterion for equilibrium fracture. Let f_c be the critical force for breaking the bonds. In the case of equilibrium crack, i.e., for quasistatic crack propagation, f_c should be related to the critical stress intensity factor K_I^c of the crystal through $f_c/a_0 \sim K_I^c \zeta^{-1/2}$ where ζ is the distance from a crack tip comparable to a_0.

First, we have tested a couple of criteria for breaking bonds in each iterative step as follows. *Model I:* "Cut the bonds on which the force exceeds f_c." *Model II:* "Cut only one bond each time. If more than one bond has stress larger than f_c, break the one which has the maximum stress, then do the relaxation processes until no breaking bond is found." For the equilibrium crack we are concerned with here, strictly speaking, these models should yield the same results. In a finite resolution of time and space, however, we found that the results strongly depend on the rule we choose. Even when δy is quite small, events might happen such that the stress exceeds the critical value on several bonds at the same time. Those events will have a significant effect on the successive processes of breaking springs as a long time memory. In this point of view, we took the latter (model II) in the preceding analysis. The rule we used here can be regarded as a limiting case of the noise reduction model which was studied previously in Ref. [13].

We can introduce a few dimensionless parameters in this model: One is the ratio of thermal diffusion length and W defined as

$$b=\beta W \ , \tag{6}$$

and the other is the externally applied force:

$$S=\alpha \Delta T E a_0/f_c \ , \tag{7}$$

where E is Young's modulus which may depend on the direction of the applied force. For the pressure parallel to a unit vector $\mathbf{n}=(n_x,n_y)$, one can easily show that

$$\frac{1}{E}=\frac{k_1+k_2}{k_1(k_1+2k_2)}+\frac{k_1-2k_2}{k_1k_2}n_x^2n_y^2 \ .$$

From the definitions, bS can be regarded as the dimensionless thermal stress applied to the specimen, therefore it should act as a control parameter in the system. The only quantity related to the time-dependent behavior of the system is the diffusion length $1/\beta$.

Computer simulations were carried out for a rectangular shape with typically 32×128 nodes. (See Fig. 1.) On the boundary of the rectangles, there is no constraint on the motion of nodes and no external pressure applied on the sides. The number of nodes in the horizontal (x) direction has been changed from 24 to 64. In the vertical (y) direction we have up to 256 nodes. As material specific constants, we choose $k_1=1$ and $k_2=0.7$, respectively. Note that there are two different types of anisotropy in this system: One is the anisotropy of the lattice itself, and the other is the elastic anisotropy which does not vanish even in the continuum limit. Changing the ratio of k_1 and k_2, one can control the elastic anisotropy

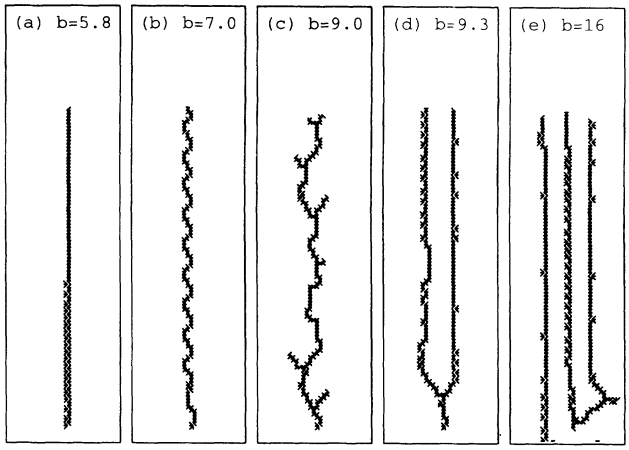


FIG. 1. Typical patterns obtained for several control parameters. Each 2D crystal consists of 32×128 nodes. $S=22.6$. Broken bonds of (a) straight ($b=5.8$), (b) oscillatory ($b=7.0$), (c) branching ($b=9.0$), (d) two-parallel ($b=9.3$), and (e) three-parallel ($b=16$) cracks are shown.

(the latter) and, as a result, preferred directions of crack propagation. If $k_1/k_2>2$, one can expect that cracks "prefer" to move in the x or y direction. Otherwise, cracks will move more easily in the oblique direction to the x and y axes. It is our future problem to investigate the influence of the elastic anisotropy on the pattern selection.

A tiny straight crack was prepared near the bottom center of the crystal as the initial crack. For small b or S, the initial crack does not grow at all. Increasing b or S, the transition from nonpropagating crack to the straight propagating crack takes place. The crack runs in the y direction near the center of the plate even when the initial position of the crack is biased from the center. For instance, when fixing $S=22.6$, the transition occurs at $b\simeq5.8$.

Increasing further those control parameters, i.e., with stronger thermal stress, the straight crack becomes oscillatory with an apparent wavelength λ. From a number of independent simulations by changing b and S we obtained the transition line which can be well represented by the curve of $bS\simeq170$ as shown in Fig. 2. The selected wave-

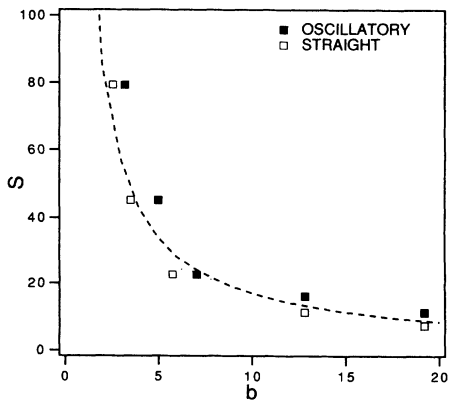


FIG. 2. Transition line of oscillatory cracks (black rectangles) from straight cracks (white rectangles) in the b-S plane. Dotted line represents the curve of $bS=170$.

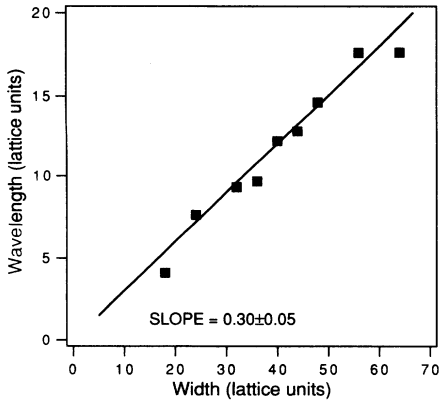


FIG. 3. Selected wavelength λ at the transition point between straight and oscillatory crack formation versus the width of crystal W.

length at the onset of the transition (see Fig. 3) is proportional to the width of plates W as

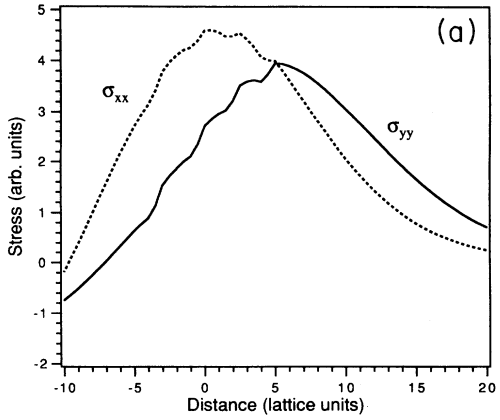
$$\lambda_c = aW, \quad a = 0.30 \pm 0.05 ,$$

which seems to be independent of other parameters. This gives very nice agreement with the experimental results ($a \simeq 0.28$) for glass plates in Ref. [4] and suggests that the isotropic characteristics of glass are not important for the oscillatory motion of crack tips. The obtained λ has a larger deviation probably because of the mismatching between lattice size and λ to be selected.

After the transition it turned out that the wave form became gradually irregular and the position of the crack tip fluctuated around the middle part of the crystal in spite of the completely deterministic calculations except for numerical errors.

For larger b or S, a single crack becomes unstable eventually, then branching of crack tips is observed. But, as seen in Fig. 1(c), there is still only one main branch spanning from bottom to top like trees. Just above the branching crack region, we find two cracks running simultaneously, dividing the plate into three parts whose widths are almost the same as each other. Furthermore, we found up to three parallel cracks by increasing the parameters. To be compared with the experimental phase diagram [4], our model would be valid, at least qualitatively, in the parameter region even for very strong thermal stress.

In the steady state of crack propagation, crack tips go at some distances l ahead of the position where the thermal gradient is maximum, i.e., at water level. In other words, the distance l is selected to make the stress at the tip marginal. In Fig. 4(a) stress at a straight crack tip is plotted by changing the vertical position of the tip for $b = 7.0$ and $S = 22.6$. To obtain this plot, a straight crack was prepared first, and then stress near the crack tip was calculated numerically for many cases of the distance between the prepared crack and the water level. Since the lattice size is not very small compared to the thermal diffusion length $1/\beta \simeq 4.5$, some tiny kinks are found in the plot as a numerical artifact, although the curve should be smooth. When l is small, which corresponds to small thermal stress, σ_{xx} is larger than σ_{yy}. On the other



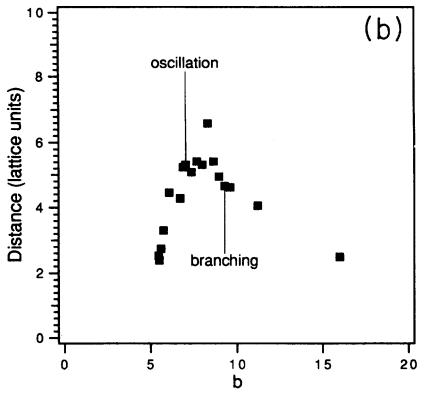


FIG. 4. (a) Numerically obtained stress σ_{xx} and σ_{yy} at the tip of the straight crack as a function of the distance l from the position of maximum thermal gradient. $b = 7.0$, $S = 22.6$. (b) Position of propagating crack versus control parameter b. $S = 22.6$.

hand, for larger l than a critical length l_c, σ_{yy} becomes dominant. As pointed out in Ref. [5], this may cause an instability for the mode I crack propagation. Accordingly, in our simulations, the transition to oscillatory region seems to take place when $l = l_{\rm osc} \simeq l_c$ as seen Fig. 4. But, unfortunately, in our very limited resolution of space we hardly compare l_c and $l_{\rm osc}$ quantitatively. When the applied thermal stress is very large, l becomes rather small since elastic energy can be dissipated by creating more than one crack tip.

We would like to mention here the simulations performed with periodic boundary conditions. In order to make the two vertical sides of the rectangular crystal identical, movement of the nodes interconnected with springs is constrained on a cylinder of radius $W/2\pi$ whose thermal expansion coefficient is zero. Thus this modeling does not represent a real three-dimensional cylindrical crystal, because the radial shrinkage is not taken into account. We obtained very similar propagating cracks including straight, oscillatory, and branching patterns as seen in free boundary cases. While oscillatory behavior of propagating cracks was also found, the selected wavelength was different and the direction of the crack was tilted with a small angle. We obtained the

wavelength $\lambda_{cyl} \simeq 0.5W$ from several runs of computer simulations. However, it is unclear why such oscillation of cracks is possible even in the periodic boundary condition which seems to give rise to no mechanism for turns of cracks. That is, considering the symmetry of the periodic boundary condition, a spiral rather than a wave would be more natural to see.

Summarizing this Rapid Communication, we have performed computer simulations of two-dimensional crack propagation by a deterministic spring network model. We found that the spring network model does work successfully for the fracture formation quasistatic cases even in a very large thermal stress region. The spring model we used here gave nice agreement with the experimental results for glass plates in the aspect of pattern selections. In particular, the wavelength of cracks at the transition between straight and oscillatory crack formation was determined by the width of a two-dimensional crystal in a linear function, which was also in accord with the experiment.

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