Maturation of crack patterns

E. A. Jagla

The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34014 Trieste, Italy
(Received 20 November 2003; published 18 May 2004)

Superficial (two-dimensional) crack patterns appear when a thin layer of material elastically attached to a substrate contracts. We study numerically the maturation process undergone by these crack patterns when they are allowed to adapt in order to reduce its energy. The process models the evolution in depth of cracks in geological formations and in starch samples ("columnar jointing"), and also the time evolution (over thousands of years) of crack patterns in frozen soils. We observe an evolution towards a polygonal pattern that consists of a fixed distribution of polygons with mainly five, six, and seven sides. They compare very well with known experimental examples. The evolution of one of these "mature" patterns upon reduction of the degree of contraction is also considered. We find that the pattern adapts by closing some of the cracks and rearranging those in the immediate neighborhood. This produces a change of the mean size of the polygons, but remarkably no changes of the statistical properties of the pattern. Comparison with the same behavior recently observed in starch samples is presented.

I. INTRODUCTION

Consider a thin layer of a solid material elastically attached to a substrate. If the material contracts (or the substrate expands), elastic stresses appear in it. When these stresses are sufficiently high, cracks can appear in the material, giving rise to a fragmentation process. Well known examples of this phenomenon are cracking on mud and paints. In these cases the water evaporation produces the contraction of the material that is responsible for cracking. In other cases, as in the cracking of ceramic coatings, it is typically the contraction upon cooling that generates the same phenomenon. Fragmentation is known to produce a two-dimensional pattern of cracks whose statistical properties have been studied experimentally [1] and theoretically [2]. With some variations depending on the particular case, these crack patterns are hierarchical structures, with younger cracks meeting older ones perpendicularly. Then most crack joints are "T" shaped [3], with the horizontal part being older than the vertical part.

There is however a small number of remarkable cases in which fragmentation crack patterns undergo a "maturation" process. This means that starting from a hierarchical pattern as described above, cracks can adapt smoothly to optimize its configuration. This optimization process is driven by the tendency of the crack pattern to reduce its mechanical (elastic plus crack) energy. Special conditions have to be fulfilled for this maturation to take place. To modify a given crack pattern, cracks should be able to displace laterally, and this implies typically the surmounting of enormous energy barriers (although the final state has lower energy than the original one). Particular conditions make this lateral displacement possible in (at least) two different cases.

One is the case of crack patterns formed on the ground of very cold regions of the earth [4], and also in other planets [5]. In this case the frozen ground (named "permafrost") cracks when the rapidly fallen temperatures of winter make the surface contract with respect to lower parts of the terrain. This first crack pattern is of the kind described above. The

cracks get filled with new ice and debris, and when temperature rises after winter the cracks tend to close. However, the new material that filled the cracks is weaker than the old permafrost, and the next year cracks open almost on top of the "scars" of first year cracks. However, small lateral variations can occur from one year to the next. There are many reasons that can make a crack to be shifted laterally in one direction or the other, from one year to the next. Most of these reasons (as, for instance, inhomogeneities in the materials) are not expected to bias the shift of the crack in one particular direction. But there is at least one reason for a crack to shift in a particular direction, and that is the tendency to reduce the energy of the crack pattern. In fact, from a statistical point of view it is reasonable to expect the crack pattern to adapt in order to reduce its energy. This tendency provides a bias for the evolution of the crack pattern in permafrost that over thousands of years is able to qualitatively modify its appearance [4]. In fact, after maturation, crack joints become more Y shaped, as this form has lower energy than the T shaped original joints.

The second, better known and more remarkable example of crack pattern maturation takes place in the case of columnar jointing. It occurs in basaltic rocks when they cool after its expulsion in a volcanic event [6], and also in desiccating starch [7] driven by the shrinkage due to humidity loss. In both realizations, a superficial pattern of cracks very much like the one described in the first paragraph first develops in the material. But here, this crack pattern penetrates the material as deeper parts of it cool (or desiccate). It is this progression into the interior that allows the maturation of the pattern to take place, now as a function of depth, reaching a polygonal structure whose further advance defines prismatic columns. In this case there is no true lateral movement of the cracks. But we will make the assumption that an effective description in terms of lateral movement can be given if we choose a reference system that moves with the penetrating crack front. The similarity between the results we will obtain and those of the true three-dimensional (3D) system will confirm that this assumption makes sense.

We use here a recently developed model of fracture [8] to describe crack patterns in a two-dimensional material elastically coupled to a substrate. In the original formulation of this model cracks have to be pinned in some way in order to avoid them to move laterally (since typically this movement is unphysical). Here instead, we take advantage of this movement (driven by the tendency to minimize the energy of the system) to observe how an originally disordered pattern becomes polygonal during its maturation. We also investigate the way in which a stable polygonal pattern is modified when the degree of contraction is modified. We observe that some individual cracks disappear (terminate, in the 3D language of columnar jointing) when contraction is reduced, giving rise to local rearrangements in the pattern. This mechanism provides a way to change the mean width of the columns as a function of depth in the basalt formations and in starch, and it has been observed to occur in this last case. We finish with a discussion on what the typical width of columns in three-dimensional formations is.

II. THE NUMERICAL MODEL

We use a technique recently developed [8] to treat fracture and cracks in the context of phase field modeling [9]. The free energy of the system is written in terms of the strain tensor $\varepsilon_{ij} \equiv 1/2(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$, with $\mathbf{u}(\mathbf{r})$ being the local displacement field. We choose the form of the free energy in such a way that it reduces to the normal elastic energy for small strains, but for large strains it is able to describe cracks. This is achieved by a saturation of the free energy of the system for large values of ε_{ij}. The inclusion in the free energy of terms proportional to gradients of ε produces a smoothing of cracks, which although artificial, is however very important to us. On one hand it makes the description isotropic and insensitive to the numerical mesh we use in the calculation (as long as the discretization is much thinner than the smoothing distance of the fracture). On the other hand it allows the cracks (that in the regularized theory could be pictorially described as "solitons") to move around the system to find configurations of lower energy. This wandering will model the maturation of the crack pattern. The free energy is taken to be rotationally invariant, in order to describe cracks in an isotropic material.

To write down explicitly the equations we actually solved in our two-dimensional geometry, we first introduce the following notation for the independent components of ε [10,11]:

$$e_1 \equiv (\varepsilon_{11} + \varepsilon_{22})/2,$$

$$e_2 \equiv (\varepsilon_{11} - \varepsilon_{22})/2,$$

$$e_3 \equiv \varepsilon_{12} = \varepsilon_{21}, \tag{1}$$

which are named, respectively, the dilation, deviatoric, and shear components. These three variables are not independent. They satisfy the St. Venant compatibility constraint [10,11]

$$(\partial_x^2 + \partial_y^2)e_1 - (\partial_x^2 - \partial_y^2)e_2 - 2\partial_x\partial_y e_3 = 0. \tag{2}$$

The free energy density is

$$F(\varepsilon) = \frac{F^0(\varepsilon)g}{[1 + F^0(\varepsilon)/f_0]}, \tag{3}$$

where

$$F^0(\varepsilon) = B(e_1 - e_1^0)^2 + \mu[(e_2 - e_2^0)^2 + (e_3 - e_3^0)^2], \tag{4}$$

and B and μ are related to the two-dimensional bulk and shear modulus of the material. $e_i^0(\mathbf{r})$ are externally controlled functions that allow us to prescribe the locally preferred state of the system, and $g(\mathbf{r})$ is another (positive) function that will be used to model some random inhomogeneities in the system. There is no particular significance in the exact form of the free energy (3), apart form the fact that it has to reduce to that of linear elasticity for small strains, and tends to a constant for large strains. The chosen form is just a simple analytical interpolation between the two limits. The limiting value f_0 of F for $\varepsilon \to \infty$ (assuming $g=1$) is related to the crack energy in the model.

Regularization of cracks is provided by a gradient term F_g in the free energy density, which we choose to be of the form

$$F_g = \sum_{i=1,2,3} \alpha_i (\nabla e_i)^2, \tag{5}$$

where we have to choose $\alpha_2 = \alpha_3$ to retain rotational invariance.

An additional ingredient that has to be added here with respect to the basic model of Ref. [8] is the inclusion of the elastic energy density F_{el} of the system attached to the substrate. In terms of the displacement variables $\mathbf{u}$, this elastic energy can be written in the form

$$\int d^2r F_{el} \equiv \gamma \int d^2r |\mathbf{u}(\mathbf{r})|^2, \tag{6}$$

where γ measures the stiffness of the interaction with the substrate. As we take the components of ε to be our basic variables, we have to recast this energy in terms of these. This can be easily done in the Fourier space, and the result is

$$\int d^2r F_{el} = \gamma \int d^2k \frac{|\tilde{e}_2(\mathbf{k})|^2 + |\tilde{e}_3(\mathbf{k})|^2}{k^2}, \tag{7}$$

where $\tilde{e}_i(\mathbf{k})$ are the Fourier transforms of the original $e_i(\mathbf{r})$. The equations of motion are taken to be of the overdamped form, namely,

$$\frac{\partial e_i(\mathbf{r})}{\partial t} = -\lambda \frac{\delta F}{\delta e_i(\mathbf{r})} (i = 1,2,3), \tag{8}$$

where

$$F = \int d^2r(F + F_{el} + F_g). \tag{9}$$

The St. Venant constraint is implemented by using a Lagrange multiplier. No thermal disorder (Langevin term) is included and then the dynamics is fully deterministic.
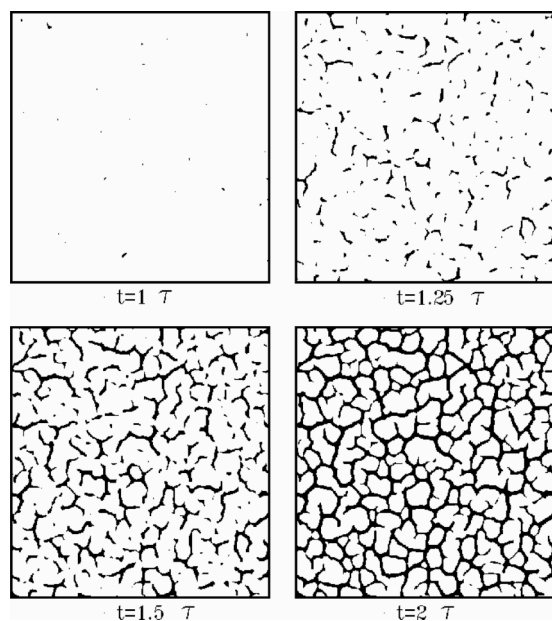
FIG. 1. Appearance of a typical fragmentation pattern during the first stage of the evolution. The time scale τ is given by $\tau^{-1} = \lambda B$. The contraction imposed is $c = 0.7$.
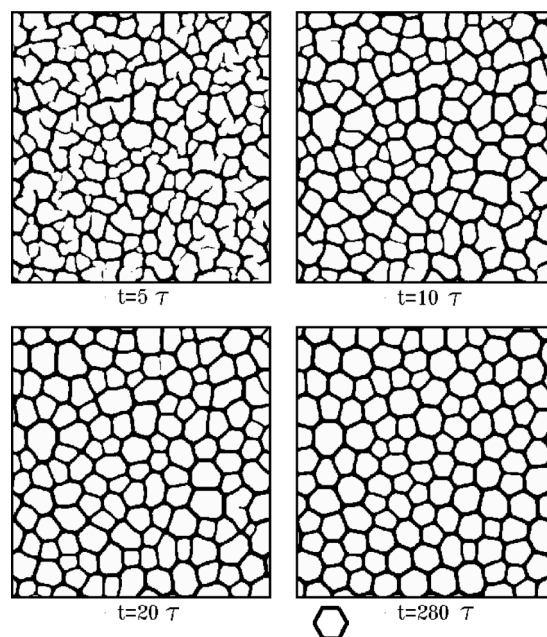

FIG. 2. Maturation of the fragmentation pattern at longer times (note the change in time intervals with respect to previous figure). The lateral displacements of cracks allow the system to reach a stable state (bottom right) which is a local energy minimum. The size of the hexagon in the perfect pattern that corresponds to the absolute minimum of the energy is indicated.

III. RESULTS

We did the simulations on a square mesh of 512×512 elements, using periodic boundary conditions. Starting from the configuration $e_1(\mathbf{r}) = e_2(\mathbf{r}) = e_3(\mathbf{r}) = 0$ we simulated a uniform and abrupt contraction of the system by taking $e_1^0(\mathbf{r}) = c$, $e_2^0(\mathbf{r}) = 0$, $e_1(\mathbf{r}) = 0$, $c = 0.7$. We introduce also a finite disorder, taking $g(\mathbf{r})$ in Eq. (3) to be a random function on the lattice, uniformly distributed between 0.75 and 1.25. We keep B and the mesh discretization δx as scale-fixing parameters, and take $\mu = 0.5B$, $\alpha_i = 0.5B \delta x^2 (i = 1, 2, 3)$, $\gamma = 0.0025B/\delta x^2$, and $f_0 = 0.5B$. Under these conditions we solve the evolution equations. We see in Figs. 1 and 2 snapshots of the time evolution of the system. The figures are done by marking the points in which $e_1 > e_{th}$, where e_{th} is some constant threshold value. To make sense, this value must be chosen in such a way that according to our definition of the free energy [Eqs. (3) and (4)], the system is intact (elastic) for $e_1 \ll e_{th}$ and broken for $e_1 \gg e_{th}$. We have chosen $e_{th} = 0.5$, and verified that the results do not change appreciablly when using $e_{th} = 1$. In this way we are basically plotting the cracks present in the system. It is important to note that due to the finite value of α_i, broken elements do not form strictly one-dimensional "strings" in the system, but they clusterize, making cracks acquire a finite width, as it is apparent in the pictures. This is a crucial point to simulate an isotropic system.

We can distinguish two different stages in the temporal evolution. During the nucleation stage (Fig. 1) cracks appear rather disorderly in the system and propagate around. The pattern that forms is very dependent on many details of the simulation, as, for instance, the amount of disorder present [namely, the values of the function $g(\mathbf{r})$]. This is the kind of pattern we have described in the Introduction as a fragmen-

tation pattern. During a second stage the maturation of the pattern occurs (Fig. 2). This is observed as a progressive lateral displacement of the cracks towards a configuration of lower energy. It is necessary to emphasize again that in standard fragmentation processes this maturation cannot take place, as cracks cannot move from their positions. In our numerical model cracks can in fact move laterally, since this does not imply the surmounting of a large energy barrier.

The lateral movement of cracks in our model is, however, rather slow compared to its nucleation, and that is why it is not seen on the time scale of the nucleation stage. We stress that we are not forcing the crack pattern to become polygonal, or cracks to terminate onto other cracks, it is the system itself that prefers this kind of configuration as this reduces its energy. The final, stable pattern is that at the bottom right of Fig. 2. It corresponds to a relative minimum of the energy of the system, the absolute minimum [for $g(\mathbf{r}) = 1$] being a perfect hexagonal pattern with a polygon size (calculated numerically with the same model) as indicated also in Fig. 2. Contrary to what happens in the nucleation stage, the evolution during the maturation process is essentially independent of the presence of inhomogeneities (and also independent of the presence of some thermal noise). We have checked this by repeating the maturation process starting from the last pattern in Fig. 1 but resetting the values of the function $g(\mathbf{r})$ in Eq. (3) to one, namely, making the system structurally homogeneous. The evolution observed in this case is equivalent to that in Fig. 2, indicating that local defects are irrelevant during the maturation stage.

The mature pattern contains mostly polygons of five, six, and seven sides, and a small number with four and eight
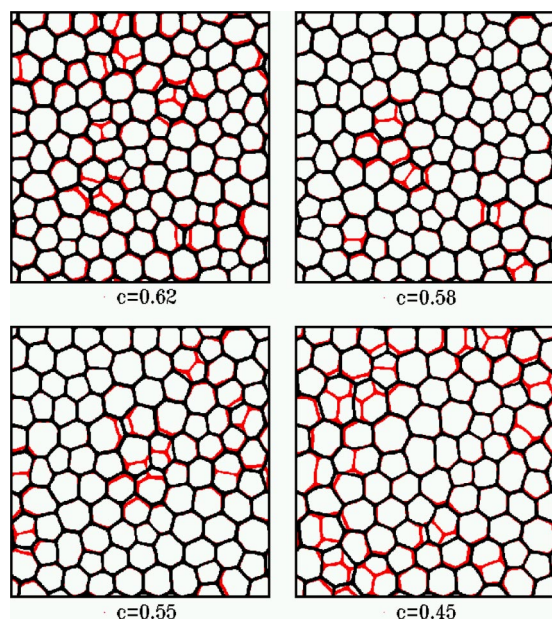
FIG. 3. (Color online) Evolution of the mature pattern of Fig. 2 (bottom right) upon reduction of the extent of contraction c. Note the disappearance of some cracks and the local rearrangement that occur. To facilitate the visualization we plot also the immediately previous pattern. For the first panel the previous pattern is the last one in Fig. 2.

FIG. 4. Evolution of the mean area A of the polygons as a function of the degree of contraction c, when c is reduced from larger to smaller values, and ideal value A^{id} of the area of polygons in the perfect hexagonal pattern that minimizes the energy of the system. There is a critical value of contraction ($c \sim 0.42$) below which the uncracked configuration is the one with minimum energy.

sides. They are statistically very similar to those in real columnar formations (see Fig. 5 below and Fig. 8 in Ref. [12]). We note that the mean area of polygons for different number of sides follows a linear relation, known as the Lewis law, after he encountered it in other two-dimensional patterns [13]. This law follows if the pattern is assumed to be maximally random [14].

The present results can be compared with those obtained previously [12] using a phenomenological model for the energy of the cracked material. The present approach is however much more general than that in Ref. [12]. Here, we are not assuming any phenomenological form of the energy as a function of the areas of the polygons, the energy of the system builds up from the free energy presented in the preceding section. In addition, crack segments are not forced here to be straight, and in fact we can see in the last panel of Fig. 2 that some of them are slightly curved. The curvature occurs particularly when there is a large difference between the areas of polygons on both sides of the crack segment, always curving it in the direction in which areas tend to be closer. The reason for this is again energetic: slightly curving a crack does not pay much crack energy, but produces a gain in elastic energy if the areas of the two adjacent polygons tend to become closer to each other. This curvature has been in fact observed to occur in a full three-dimensional calculation for a simple geometry [15].

An interesting problem to be investigated with the present model is the way in which a stable polygonal pattern changes when there are changes in the parameters that control the extent of contraction. As an outcome of this analysis we will get an idea of the expected evolution of the patterns down in the columnar formation (after the first maturation), since the
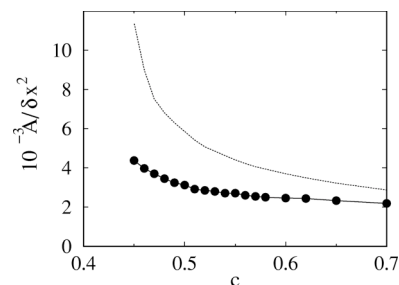
thermal stresses in deeper parts of the material are lower than close to the surface. Since a lower grade of contraction corresponds to an ideal pattern with larger polygons, we may wonder what is the way (if any) in which one of our patterns adapts to the new conditions. We present in Fig. 3 the results of simulations when the extent on contraction c is reduced. We see that there is an increase in the mean area of the polygons when c is reduced. The area increase is not homogeneous over all polygons, but occurs due to the disappearance of particular crack segments, merging two (or three) adjacent polygons into one. After the disappearance of the crack segments there is a local rearrangement of the pattern which adjusts to the new configurations. Those regions in which no crack disappear remain perfectly stable despite the change in the contraction.

The evolution of the mean area A of the polygons as a function of c is shown in Fig. 4 along with the ideal area A^{id} of the hexagons in the perfect hexagonal pattern of minimum energy. We see that the evolution tends to follow that of the ideal structure, although A is always smaller than A^{id} [16]. We note also that in the present model there is a critical value of c (~ 0.42) for which A^{id} diverges, and we expect the same occurs for nonideal patterns. This happens because the elastic energy per unit area gained when generating a polygonal crack pattern decays very rapidly when the size of the hexagons increases sufficiently. The sum of this elastic energy plus fracture energy may not have a minimum with respect to the area of polygons if the degree of contraction c is too small. Note that the same does not apply to a real three-dimensional columnar case (see the following section).

It is remarkable that the statistical properties of the pattern do not change appreciably during this relaxation stage. In Fig. 5 we see that despite a change in the mean area by more than 50%, statistical distribution of polygons by number of sides and areas remains constant within numerical fluctuations associated to the finite size of the system [17]. Note that it is precisely the "imperfection" of the crack pattern that makes possible the adaptation of the mean area to a condition of lower contraction. For a perfect hexagonal pattern it is impossible to find a way to adapt the pattern slightly and obtain another hexagonal pattern with slightly larger polygon area. In our case the mean area of the pattern is increased by making some crack segments between polygons disappear.
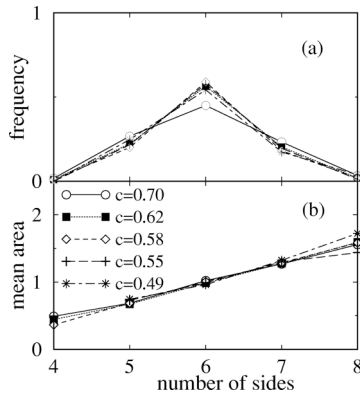
FIG. 5. (a) Frequency of polygons with different number of sides and (b) mean area of polygons with different number of sides (normalized to the mean area of all polygons) for patterns obtained by reducing c.

IV. THE PROBLEM OF THE TYPICAL COLUMN WIDTH IN COLUMNAR FORMATIONS

The two-dimensional model we have studied is perfectly well defined, and provides values for the size of the polygons in the ideal hexagonal pattern that minimizes the total energy of the system. We want to comment at this point to what extent these two-dimensional results can be applied to the full three-dimensional columnar problem. For a straightforward application to be possible, the elastic energy stored in a columnarly cracked three-dimensional material should be stored in a layer around the crack front of thickness w, in such a way that w is much smaller than the typical column width l ($l \sim A^{1/2}$). If this is satisfied, the two-dimensional description is directly applicable. The only consideration to be made is that two-dimensional variables have to be scaled from the three-dimensional variables using w. For instance, the effective crack energy per unit length η and elastic constants B and μ of the two-dimensional description are obtained from the real three-dimensional values as $w\eta^{(3D)}$, $wB^{(3D)}$, and $w\mu^{(3D)}$. Unfortunately the condition $w \ll l$ is never satisfied. In fact, the elastic energy of a columnar formation is stored in a portion of thickness $w \gtrsim l$ around the crack front [18]. The coincidence of the statistical properties of our two-dimensional patterns and those in true three-dimensional cases indicates that these properties are robust with respect to this difference. However, the calculation of the ideal size of the perfect hexagonal pattern (and then an estimation of the typical size of nonperfect real patterns) has to be reconsidered for the three-dimensional case. In fact, in our two-dimensional model, in which a layer of material is attached to a substrate, there is an ideal hexagonal pattern of well-defined polygon size that minimizes the energy of the system. The application of the same principle of minimizing the *total* energy leads in the three-dimensional case to nonsense: the contribution of the fracture energy to the total energy is always much larger than the elastic contribution. A minimum can only be obtained with no cracks at all.

The correct way to pose the problem of the typical size of the polygons in three dimensions is the following: in the three-dimensional case, we have a temperature profile that we assume to be dependent only on depth z, passing more or less steeply from T_0 at $z \to -\infty$ to $T_1 > T_0$ at $z \to \infty$, in such a way that a temperature front can be defined. At time $t=0$ the temperature front is assumed to be located at $z=0$. We will consider the idealized case in which the temperature profile is rigidly displaced towards the interior as a function of time, with some fixed velocity v, namely, $T(z,t)=\widetilde{T}(z-vt)$. We assume that a stable polygonal pattern of fractures has formed, and that its front is located at some depth z_0, which moves down locked to the temperature profile, namely, $z_0=z_r+vt$, where z_r measures the relative position of the crack pattern and the temperature profile. The value of z_r depends mainly on the typical size of the pattern l and the overall temperature difference $\Delta T=T_1-T_0$. A previous stability analysis has shown in a simplified case [18] that under the present conditions, patterns with different l can propagate in a stable manner, with z_r being a decreasing function of l, namely, larger patterns are more retarded with respect to the temperature front. However there is a limit to this stable propagation. If l or ΔT are too small, the crack front becomes unstable: not all cracks can propagate. It is tempting to argue (and this is also based upon what is observed in three-dimensional starch samples, see below) that in this case some crack segment will remain halted, and the rest of the pattern propagates. In this way l is effectively increased and the crack front becomes closer to the temperature front, in such a way that the new pattern is now stable. In a situation in which ΔT decays smoothly with time (whereas at the same time the front penetrates the material), we may expect that the pattern will always be located at the value z_{cr} that marks the limit between stable and unstable propagation. This is the condition that determines the size of the columns in terms of the temperature profile, the elastic properties of the material and the crack energy. For the case of a sharp temperature jump and generalizing the two-dimensional expressions for elastic and fracture energy in Ref. [18], we obtain that the crack front is located precisely at the border between stable and unstable regions when $B(\alpha\Delta T)^2 l/\eta$ is some constant value k of order unity (this value is not easy to calculate). Here α is the thermal expansion coefficient and B is a typical elastic constant of the material. From here we obtain the typical width of the columns as

$$l = k\frac{\eta}{B}(\alpha\Delta T)^{-2}. \tag{10}$$

The typical size is then positively correlated to the crack energy and negatively correlated with the elastic stiffness of the material, both facts being qualitatively reasonable. The size l is also proportional to the negative second power of the temperature jump responsible for cracking. We should keep in mind, however, that this result is valid only for the assumed sharp step form of the temperature profile. In other cases we should search for the critical position of the crack front z_{cr} along the lines used in Ref. [18]. Note that $\alpha\Delta T$ plays in three dimensions the role of the degree of contraction c in our simulations. The preceding formula indicates that the typical size of polygons diverges only when $\alpha\Delta T \to 0$, contrary to the critical value of c we found in two

dimensions (see Fig. 4). This would indicate that if the driving force for cracking is slowly reduced when going deeply into the material (as may occur due to the higher difficulty to expel heat—or humidity in starch—through the upper material) the size of the pattern should adapt by increasing their typical size, but it would never stop abruptly.

Recent tomography experiments in starch samples [19] show that termination and rearrangement of cracks seem to be in fact the main mechanism by which the polygonal pattern evolves in depth. In starch samples the humidity gradients are expected to be reduced when going deeper into the sample, and that is why the typical width of the columns tends to increase. However, a quantitative verification of a relation such as Eq. (10) (or the equivalent one for a more realistic time dependent temperature or humidity profile) is not possible at present as it would require the in situ determination of the temperature profile under which the cracks form, and not only the observation *a posteriori* of column thickness as a function of depth.

V. CONCLUSIONS

We have studied numerically the formation and maturation process of a two-dimensional crack pattern that is allowed to adapt to find configurations of minimum energy. The original cracks appear in a rather disordered way, but the pattern naturally evolves towards a polygonal configuration with well defined statistical properties. We argue that this maturation process occurs in crack patterns on the ground of arctic regions (permafrost) and effectively in the columnar jointing of basalts and starches, as a function of depth. Our model allows also to study the evolution of mature polygonal patterns when the extent of contraction is reduced. We have found that in this case the pattern adapts by closing ("terminating" in the three-dimensional interpretation) some cracks and rearranging those cracks in the immediate neighborhood. This evolution has been recently observed to occur in starch samples. Although it does not contain all features of the full three-dimensional problem, our approach produces patterns of very good statistical agreement with real ones. The issue of the typical scale of the three-dimensional pattern is beyond the reach of the two-dimensional model, and we have provided for this case a plausible description that relates the typical size of the polygons with the elastic and thermal properties of the material, and with the details of the temperature profile.

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[16] This difference can be reasonably considered to be a consequence of the metastabilities in the process we are simulating. In fact, if at some point we revert the evolution of contraction, making now c increase, we have observed the nucleation of new crack segments, typically bisecting the largest polygons. In this evolution the values of A we get are *larger* than A^{id}, namely, the evolution of A as a function of c has a strong hysteresis that encloses the ideal value corresponding to the ideal energy minimum.

[17] In Fig. 5(a), it seems that the first stable pattern (with the original value of contraction $c=0.7$) is slightly different to the rest, having less polygons with six, and more with five and seven sides. We cannot tell at this point if this is systematic or associated to statistical fluctuations.

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