Nucleation of interfacial shear cracks in thin films on disordered substrates

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Abstract. We formulate a theoretical model of the shear failure of a thin film tethered to a rigid substrate. The interface between film and substrate is modeled as a cohesive layer with randomly fluctuating shear strength/fracture energy. We demonstrate that, on scales large compared with the film thickness, the internal shear stresses acting on the interface can be approximated by a second-order gradient of the shear displacement across the interface. The model is used to study one-dimensional shear cracks, for which we evaluate the stress-dependent probability of nucleation of a critical crack. This is used to determine the interfacial shear strength as a function of the film geometry and statistical properties of the interface.

Keywords: fracture (theory), heterogeneous materials (theory)
1. Introduction

In this study we investigate the interfacial failure of thin films subjected to shear loads. Besides obvious applications to materials problems such as shear failure and/or abrasive wear of coatings and shear-induced delamination of thin films, the problem at hand has some interesting applications in geosciences, where models similar to the one studied in this paper have been applied to the initiation of snow slab avalanches and landslides [1]–[3].

Most of the mechanics literature on interface failure has focused on the static and dynamic properties of pre-existing interface cracks in systems where the interface and the surrounding material have known, space-independent material properties. In the present investigation, on the other hand, we study the problem of crack nucleation under load in situations where the interface with the substrate is disordered, such that interfacial shear strength and fracture energy are random functions of position. Failure of disordered interfaces has been studied mainly in the statistical physics community, usually using idealized ‘concept models’ such as fiber bundle models with phenomenological load sharing rules (see e.g. [4, 5]). From a statistical physics point of view, failure of disordered interfaces is an interesting topic because it allows one to investigate the more general problem of failure of three-dimensional disordered media (for an overview, see [6]) in a setting of reduced dimensionality. This removes some of the complications that are associated with the dynamics of non-planar cracks such as two-dimensional crack front roughening and emergence of rough fracture surfaces [7, 8], and with the anisotropic interactions that govern damage accumulation and crack screening in bulk solids [9].

Cracks along interfaces below or between thin elastic plates have been investigated mainly in view of crack pinning, crack front roughening and crack propagation [10, 11]. The problem of interface crack nucleation, on the other hand, has received little attention despite its obvious importance for assessing the strength of interfaces which do not contain pre-existing cracks or notches. Interface crack nucleation in a bulk material was studied by Arndt and Nattermann [12]. These authors do not explicitly envisage interface failure but consider a linear crack in a two-dimensional system. This is tantamount to assuming...
the existence of a weak interface, since otherwise the emerging crack will roughen two-dimensionally [8]. In the present study we carry out a similar investigation for shear cracks in a weak interface between a thin elastic film and a rigid substrate. We evaluate the crack nucleation probability as a function of stress, geometry, and statistical parameters characterizing the interface. We then use a weakest-link argument to deduce the failure stress distribution and to evaluate the size dependence of the system strength. The theoretical arguments are validated by comparison with numerical simulations.

2. Formulation of the model

We consider a thin elastic film of thickness $D$ tethered to a rigid substrate. The interface with the substrate is modeled as a cohesive layer in the plane $z = 0$. The response of the interface to shear loads is characterized by a scalar stress–displacement relationship $\sigma_{xz}(x, z = 0) = \tau(u(x))$ where $\sigma_{xz}$ is the shear stress at the interface, $\tau$ is the interfacial shear strength, and $u(x) = w_x(x, z = 0)$ is the shear displacement across the interface.

The film is loaded in plane shear by spatially homogeneous tractions applied to its free surface at $z = D$, giving rise to a space-independent ‘external’ shear stress $\sigma_{xz}^{\text{EXT}}$. The maximum stress that can be supported by the interface is denoted as $\tau_M$, and the failure energy is given by the integral

$$ w_f = \int \tau(u) \, du =: \tau_M u_0, $$

where $u_0$ denotes the characteristic displacement to failure. Stress–displacement relationships are schematically shown in figure 1 for the semi-brittle (full line) and brittle (dashed line) cases.

Structural disorder is introduced into the model in terms of statistical variations of $\tau_M$ which is considered a stochastic process with prescribed statistical properties that will be specified later.
To analyze crack nucleation and propagation, we have to evaluate the internal stresses associated with the interfacial displacement field \( u(x) \). The elastic energy functional associated with a generic displacement vector field \( \mathbf{w}(\mathbf{r}) \) is given by

\[
H(\mathbf{w}) = \frac{\mu}{2} \int \left[ \alpha (\text{div} \, \mathbf{w})^2 + (\text{curl} \, \mathbf{w})^2 \right] d^3 r, \tag{2}
\]

where \( \alpha = (2 - 2\nu)/(1 - 2\nu) \) and \( \nu \) is Poisson’s number. Energy minimization gives the equilibrium equation

\[
\nabla^2 \mathbf{w} + \frac{1}{1 - 2\nu} \text{grad}(\text{div} \, \mathbf{w}) = 0. \tag{3}
\]

We solve equation (3) in Fourier space, imposing along the \( z = 0 \) plane the boundary conditions \( w_x(x, z = 0) = u(x), \ w_y = w_z = 0 \). This gives

\[
\mathbf{w} = \int \frac{dk}{2\pi} \begin{pmatrix} 1 - \eta k z \\ 0 \\ -i\eta k z \end{pmatrix} \exp[ikx - kz]u(k), \tag{4}
\]

where \( u(k) \) is the Fourier transform of \( u(x) \) and \( \eta = 1/(3 - 4\nu) \). We now make the crucial assumption that the film thickness \( D \) is much smaller than the characteristic length of variations in the displacement field, such that \( |kz| \ll 1 \) for all \( z \leq D \). The displacement field is then approximately given by

\[
\mathbf{w} = \int \frac{dk}{2\pi} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \exp[ikx - kz]u(k). \tag{5}
\]

Inserting this into equation (2) and using again that \( kD \ll 1 \) gives

\[
H(u) = \mu D \int \frac{dk}{2\pi} \left[ \frac{1 + \alpha}{2} k^2 \right] u(k)u(-k), \tag{6}
\]

or, in spatial coordinates,

\[
H(u) = \frac{1 + \alpha}{2} D \mu \int \left( \frac{\partial u}{\partial x} \right)^2 dx. \tag{7}
\]

The total energy of the system is obtained by adding to the elastic energy \( H \) the work done by the shear stresses at the interface:

\[
G(u) = - \int dx \left[ \int_0^{u(x)} (\sigma_{zz}^{\text{EXT}} - \tau(u)) \, du \right]. \tag{8}
\]

Minimizing the total energy functional \( E(u) = G(u) + H(u) \) leads to the equilibrium condition

\[
I \frac{\partial^2 u}{\partial x^2} + \sigma_{zz}^{\text{EXT}} - \tau(u) \leq 0, \tag{9}
\]

where the gradient coefficient is given by \( I = D \mu (1 + \alpha) \). Equations of this type have been studied by Aifantis and co-workers in the context of shear and slip bands in metal plasticity (see e.g. [13]). It may be noted that in these cases the constitutive relation contains a strain variable (shear strain or equivalent strain) in place of the displacement variable \( u \) in equation (9). The mathematical structure is, however, the same as in the present problem.
3. Energy of a shear crack and critical crack size

We first consider interfaces with space-independent fracture toughness. This serves to provide some relations and introduce notation that will prove useful in our subsequent analysis of the disordered system. We assume that a mode-II crack of finite length exists along the interface. Such a crack is characterized by a displacement field which, for \( x \to \infty \), starts from a value \( u_0 \) on the left stable branch of the \( \tau(u) \) curve, goes through a maximum \( u_1 \) which without loss of generality we assume at \( x = 0 \), and then reverts to \( u_0 \) for \( x \to -\infty \). The derivation of the corresponding solutions of equation (9) has been discussed elsewhere [3]. In the limit of long cracks (small stresses) we find that the displacement profile is approximately parabolic,

\[
u(x) = \frac{(l^2 - x^2)\sigma_{zz}^{\text{EXT}}}{2l}, \tag{10}\]

where the parameter \( l \) defines the crack length. This equation describes the displacement profile as long as \( u \gg u_0 \) such that the shear strength \( \tau(u) \approx 0 \) along the length of the crack. The parabolic profile is complemented by two boundary layers where the shear strength \( \tau(u) \) goes through the curve depicted in figure 1. For a long crack the contribution of these boundary layers can be neglected, and the energy is approximately given by

\[
E(l) \approx -\frac{l^3}{3I}(\sigma_{zz}^{\text{EXT}})^2 + 2w_\ell l. \tag{11}\]

This energy has a saddle point at the critical crack length \( l_c = \sqrt{2w_\ell I/\sigma_{zz}^{\text{EXT}}} \). Cracks above this length are unstable under the load \( \sigma_{zz}^{\text{EXT}} \) and lead to interface failure. The energy required to create a critical crack is \( E_c = 4w_\ell l_c/3 \), i.e., it decreases in inverse proportion with the applied stress. However, the barrier is always finite and, as emphasized by Arndt and Nattermann [12] for the case of bulk cracks, at physically meaningful stress levels the typical crack nucleation energies are many orders of magnitude above typical thermal energies. Hence, crack nucleation cannot occur as a result of thermally activated processes. However, energy barriers may be substantially reduced or even eliminated at certain locations due to the influence of structural disorder. In the following we analyze the conditions under which crack nucleation may occur spontaneously in a disordered medium.

4. Shear crack nucleation at a disordered interface

A disordered interface can be described in terms of a randomly varying peak shear strength \( \tau_M(x) \) or, equivalently, failure energy \( w_\ell(x) \). In this case, the energy expression, equation (11) modifies to

\[
E(l) \approx -\frac{l^3}{3I}(\sigma_{zz}^{\text{EXT}})^2 + \int_{-l}^{l} w_\ell(x) \, dx = \int_{-l}^{l} [w_\ell(x) - F(x)] \, dx, \tag{12}\]

where \( F(x) = (x\sigma_{zz}^{\text{EXT}})^2/(2I) \) is the effective driving force acting on the edge of a crack of length \( x \).

A sufficient criterion for spontaneous nucleation of a propagating shear crack starting from the position \( x = 0 \) is given by \( (\partial E/\partial l) < 0 \\forall l \) or, equivalently, by \( F(l) > w_\ell(l) \\forall l \). To
estimate the probability for this to happen, we consider the case of short-range correlated disorder where the failure energy variations can be characterized by a finite correlation length $\xi$. We split the interface into segments of length $\xi$ and treat the shear strengths in each segment as independent, identically distributed random variables with probability distribution $P(w)$. The condition that the crack can advance across the $n$th segment is $F(n\xi) > w_f(n\xi)$, the probability for this is $P(F(n\xi))$, and the crack nucleation probability is $W_{nucl} = \prod_n P(F(n\xi))$. Taking the logarithm and reverting to continuous variables, we obtain

$$\ln W_{nucl} = \frac{1}{\xi} \int \ln P(F(x)) \, dx. \quad (13)$$

To evaluate this probability we have to specify the probability distribution which characterizes the variations of interfacial strength. We assume a Weibull distribution with characteristic failure energy $w_0$ and modulus $\beta$:

$$P(w) = 1 - \exp\left(-\left(\frac{w}{w_0}\right)^\beta\right). \quad (14)$$

The mean failure strength is then given by $\langle w_f \rangle = w_0 \Gamma(1 + 1/\beta)$ where $\Gamma(x)$ denotes the Gamma function, and the coefficient of variation (COV = variance/mean) of the distribution is calculated as $\text{COV} = [\Gamma(1 + 2/\beta)/(\Gamma(1 + 1/\beta))^2 - 1]^{1/2}$.

Using the driving force given above, the crack nucleation probability is then evaluated as

$$\ln W_{nucl} = \frac{1}{\xi} \int \ln P(F(x)) \, dx = \frac{l_c}{\xi} \frac{1}{\Gamma(1 + 1/\beta)} \int \ln[1 - \exp(-s^{2\beta})] \, ds = -\frac{\sqrt{2\langle w_f \rangle I}}{\xi \sigma_{zz}^{\text{EXT}}} g(\beta), \quad (15)$$

where $s = x/l_c$ is the ratio between the crack size and the size of a deterministic critical crack. Hence we obtain that

$$W_{nucl} = \exp\left[-g(\beta) \frac{\sqrt{2\langle w_f \rangle I}}{\xi \sigma_{zz}^{\text{EXT}}} \right] = \exp\left[-\frac{E_C}{k_B T_{eff}}\right]. \quad (16)$$

This has the structure of an Arrhenius equation where the activation energy is the energy of a critical crack in the system without disorder. The place of temperature is taken by an effective ‘disorder temperature’ which depends only on statistical parameters characterizing the random field $w_f(x)$ but not on the elastic properties of the system or on the external stress. For large $\beta$, i.e. in the limit of small disorder, we may approximate the integrand in equation (15) by $\ln s^{2\beta}$ for $s < 1$, and by 0 for $s > 1$. In physical terms, this means that in this limit only crack sizes up to the critical one significantly affect the nucleation probability, which is thus tantamount to the probability of forming a critical ‘deterministic’ crack. We then simply obtain that $g(\beta) = 2\beta = \pi/(\sqrt{6} \text{COV})$, and the effective ‘disorder temperature’ becomes

$$k_B T_{eff} = \frac{4\xi \langle w_f \rangle}{3g(\beta)} = \beta \rightarrow \frac{4\xi \langle w_f \rangle}{\sqrt{6} \pi} \text{COV.} \quad (17)$$
In this weak-disorder limit the ‘disorder temperature’ is directly proportional to the variance of the Weibull distribution times the correlation length of the strength variations.

Nucleation of a propagating crack implies system failure. However, equation (16) cannot be directly interpreted as a system failure probability: while equation (16) is evaluated under the assumption that the crack starts from the origin, nucleation from any other position would produce a similar result. There are \( N = L/\xi \) potential nucleation sites in a system of length \( L \), and system failure occurs when a crack nucleates at the weakest of these. To evaluate the failure stress distribution, we use an argument from extreme order statistics. Interpreted as a function of stress, \( W_{\text{nucl}}(\sigma^{\text{EXT}}) \) gives the probability that the system has, at any stress larger than \( \sigma^{\text{EXT}} \), produced a propagating crack starting from a given nucleation site. \( 1 - W_{\text{nucl}}(\sigma^{\text{EXT}}) \) is the probability that this has not yet happened, and \( [1 - W_{\text{nucl}}(\sigma^{\text{EXT}})]^N \) is the probability that the system as a whole is still intact at the stress \( \sigma^{\text{EXT}} \). Hence we write the system failure probability as

\[
P(\sigma^{\text{EXT}}) = 1 - [1 - W_{\text{nucl}}(\sigma^{\text{EXT}})]^N \tag{18}
\]

or

\[
P(\sigma^{\text{EXT}}) = 1 - \exp[N \ln(1 - W_{\text{nucl}})]. \tag{19}
\]

For large systems, the nucleation probability at each site will be quite small, and we can therefore use the approximation \( \ln(1 - W_{\text{nucl}}) \approx -W_{\text{nucl}} \) to obtain (up to logarithmic corrections in the exponent)

\[
P(\sigma^{\text{EXT}}) = 1 - \exp \left[ - \exp \left( -g(\beta) \frac{\sqrt{2(w_f)}I}{\xi \sigma^{\text{EXT}}} + \ln(N) \right) \right]. \tag{20}
\]

This expression can be interpreted as the distribution of system failure stresses. Reciprocal failure stresses are Gumbel distributed, and the characteristic failure stress (e.g. the median of the failure stress distribution) scales as

\[
\sigma^{\text{EXT}}_{\text{xx}} \propto g(\beta) \frac{\sqrt{2(w_f)}I}{\xi \ln(N)}. \tag{21}
\]

This stress decreases logarithmically with system size. It is interesting to compare this relationship with the deterministic failure stress of a system containing a crack of length \( l \): \( \sigma^{\text{EXT}}_{\text{xx}} = \sqrt{2w_f}I/l \). It is evident that, in equation (21), the correlation length of the disorder plays a very similar role to the crack size in case of an interface without disorder.

5. Comparison with simulation results

To test the above theoretical calculations, we use a lattice automaton technique where we evaluate the displacements at discrete sites \( x_i \) on a one-dimensional lattice with lattice constant \( \xi \). Accordingly, we replace \( u_{xx} \) in equation (9) by the corresponding discrete second-order gradient. Furthermore we approximate the strength–displacement characteristics by a piecewise linear curve as shown by the dotted line in figure 1. Non-dimensional variables are defined through

\[
T = \frac{\tau}{\langle \tau_M \rangle}, \quad S = \frac{\sigma^{\text{EXT}}_{\text{xx}}}{\langle \tau_M \rangle} = U = \frac{u}{u_0}, \quad X = \frac{x}{\xi}. \tag{22}
\]
such that the average peak strength and fracture energy are by definition equal to 1. In these coordinates the equilibrium equation reads

\[ J \frac{\partial^2 U}{\partial X^2} + \Sigma - T \leq 0, \]  

(23)

where the interaction constant \( J \) is given by \( J = \left( I u_0 \right) / \left( \tau_M t^2 \right) \). The length of a critical crack in a homogeneous system is in non-dimensional coordinates given by \( L_c = \sqrt{2J/\Sigma} \), and the failure strength distribution of the disordered system, equation (20), reads

\[ P(\Sigma) = 1 - \exp \left[ - \exp \left( -g(\beta) L_c(\Sigma) + \ln(N) \right) \right] \]

\[ = 1 - \exp \left[ - \frac{g(\beta) \sqrt{2J}}{\Sigma} + \ln(N) \right]. \]  

(24)

In our simulations, random values for the local peak strengths are generated as Weibull distributed random fields with average 1, spatial correlation length 1 and Weibull parameter \( \beta \). Note that the parameter \( \beta \), together with the interaction constant \( J \) and the system size \( N \), are the only independent parameters of the problem.

The system is slowly loaded by increasing the external stress \( \Sigma \) from zero in small steps until sites become unstable as the local (external plus internal) stress exceeds the local shear strength. The displacement at all unstable sites is then increased by a small amount \( \Delta U \). New internal stresses are computed for all sites and it is checked again where the sum of external and internal stresses exceeds the local strength. The displacement at the now unstable sites is further increased, and the process is repeated until the system has reached a new stable configuration. Then the external stress is increased again and so on until the system has failed completely (\( U > 2 \) for all sites). The corresponding critical stress is recorded, and the procedure is repeated for different realizations.

Figure 2 shows a failure stress distribution determined for \( J = \beta = 1 \) in a system of size \( N = 100 \). Fitting the functional form of equation (24) by using \( g(\beta) \sqrt{2J} \) as a fit parameter yields \( g(\beta) = 2.12 \) as compared to \( g(\beta) = 1.64 \) obtained by direct computation. The discrepancy is acceptable in view of the approximations made in the derivation of the failure stress distribution. Using the same parameters, the size dependence of the mean failure stress is reasonably well reproduced without additional fitting (inset in figure 2).

Figure 3 shows the dependence of the mean failure strength on the value of the interaction coefficient and on the degree of disorder. As seen in the main graph, the decrease of strength with increasing disorder (increasing COV/decreasing \( \beta \)) is in the large-disorder regime well described by the theory. For the regime of small disorder, the theory predicts a diverging strength whereas the simulation for zero disorder yields a finite strength of 1. This is due to the finite value of the maximum stress that can be sustained by the interface; at this point the system fails by homogeneous yielding rather than by crack nucleation (for ideally brittle behavior the maximum stress would be infinite). The effect can possibly be taken into account by accounting, in the derivation of the crack properties, for a finite process zone size as discussed by Bazant [14].

According to the theory, the characteristic failure stress is expected to scale as \( \Sigma \propto g(\beta) \sqrt{2J}/\ln(N) \). The inset shows that failure stresses determined for different system sizes and Weibull exponents indeed collapse when scaled by \( g(\beta)/\ln N \) and plotted versus \( J \), even though the fit function yields an exponent of 0.38 rather than 0.5. This
Figure 2. Main graph: failure stress distribution, parameters: $J = \beta = 1, N = 100, 1000$ simulations; full line: theoretical fit using equation (24); the fit yields $g(\beta)\sqrt{2J} = 3.00$. Inset: size dependence of the mean failure stress, parameters $J = \beta = 1$; full line: $1/\Sigma = \ln(N)/3 + 1$.

discrepancy is attributed to logarithmic correction terms neglected in our derivation of the failure strength distribution.

6. Discussion and conclusions

We have derived an analytical expression for the nucleation probability of one-dimensional cracks in a disordered interface between a thin film and a rigid substrate. The method that we used is a variation of the method used by Arndt and Nattermann [12] for deriving the nucleation probability of bulk cracks. Accordingly the relations obtained have strong structural similarities with those found in [12]. A main difference between the present problem and the one treated by Arndt and Nattermann resides, however, in the nature of the elastic interactions. Elasticity is essentially non-local for a bulk crack whereas, in the present case, the small thickness of the film leads to an effectively local stress redistribution. From this point of view, our model may be considered a continuum version of local load sharing (LLS) fiber bundle models. Failure probability distributions for such models have been derived by several authors (see e.g. [15] and references therein). For certain types of disorder, such as a binary strength distribution, exact results can be obtained which confirm the existence of a logarithmic size effect. The present treatment, which uses extreme order statistics to obtain an expression for the size-dependent probability of system failure, is much more approximative. However, it has the advantage that the methods used can be applied to a broad class of local strength distributions. One may therefore ask to what extent the specific form of equation (16) is contingent on the choice of the local strength distribution: The Arrhenius-type expression, equation (16), allows us to express the crack nucleation probability in terms of the ratio between the deterministic saddle point energy and a ‘disorder temperature’ that depends
only on statistical parameters characterizing the local strength field $w_f(x)$. Is this possible only for Weibull distributed local strengths, or can similar expressions be obtained for a broader class of distributions?

To shed some light on this question, we consider an alternative strength distribution with non-continuous support which has been studied extensively in the context of LLS fiber bundle models, namely the binary distribution where the local strength takes with probability $p$ the value $w_f = 0$ and with probability $(1-p)$ the value $w_f = \langle w_f \rangle / (1-p)$:

$$P(w_f) = \begin{cases} 
0, & w_f < 0, \\
c, & 0 \leq w_f < \langle w_f \rangle / (1-p), \\
1, & \langle w_f \rangle / (1-p) < w_f.
\end{cases}$$

This distribution may be considered a simple model of a porous interface. The mean strength is $\langle w_f \rangle$, and the coefficient of variation depends on the ‘porosity’ $p$ according to $\text{COV} = \sqrt{p/(1-p)}$. Going through the steps leading to equation (16) is straightforward:

$$\ln W_{\text{nucl}} = \frac{1}{\xi} \int \ln P(F(x)) \, dx = \frac{l_c}{\xi} \int_0^{(1-p)^{-1/2}} \ln p \, ds = -\frac{l_c}{\xi} g(p),$$

where $g(p) = -\ln p / \sqrt{1-p}$. Accordingly, the nucleation probability can be written in the Arrhenius form of equation (16), with the effective temperature now given by

$$k_B T_{\text{eff}} = \frac{4\xi \langle w_f \rangle}{3g(p)} \to_{p \to 0} \frac{4\xi \langle w_f \rangle}{6\ln(1/\text{COV})}.$$
This expression is formally almost identical to equation (17) but the functional dependence on COV is different. Hence, although the formal structure of an Arrhenius equation with disorder-dependent temperature can be obtained irrespective of the details of the strength distribution, the relationship between the ‘disorder temperature’ and the parameters characterizing the variability of local strengths (here the coefficient of variation) is non-universal even in the weak-disorder limit.

The present investigation uses several important simplifications that may restrict the generality of our findings. (i) We treat crack nucleation in a single-crack approximation, i.e., we neglect the possible coalescence of cracks nucleating at different sites. Strictly speaking, this approximation is valid only in the limit of very large system sizes. In this limit, the failure stresses are low, and as a consequence the nucleation probability of a crack of any length at a given point is small. Hence, the probability of nucleating more than one crack within an interval of the order of \( l_c \) becomes so small as to be negligible, and one is effectively dealing with a single-crack problem. However, it is remarkable that the expressions which we derive in the single-crack approximation do a reasonable job in describing the simulation results even for moderate to small system sizes (figure 2). (ii) Our investigation focuses on one-dimensional cracks. This is a major restriction since in one dimension the crack shape does not depend on the disorder. In two dimensions, on the other hand, the crack shape may adjust to the strength fluctuations. In this case, the configuration space for crack nucleation becomes much more complicated as the problem can no longer be treated in terms of the crack length only, which in the present work serves as a single reaction coordinate. Instead, an investigation of crack nucleation and propagation in two dimensions requires consideration of the interplay between disorder and crack front elasticity, and a treatment of the ensuing crack front roughening. These aspects will be considered in a future publication.

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