Roughness effects on the critical fracture toughness of materials
under uniaxial stress

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The Griffith criterion is applied for the calculation of the critical fracture toughness upon which the
formation of a rough self-affine crack (which is characterized by the rms roughness amplitude \( \sigma \), the
correlation length \( \xi \), and the roughness exponent \( H \)) commences. For large crack sizes \( R \gg \xi \), the
stress field singularity close to the crack tip involves the value \( \sim 1/2 \) in both the strong and weak
roughness limit. In the latter limit, the fracture toughness \( K \) remains close to the classical value
\( K \sim 2(\gamma E)^{1/2} \) with \( \gamma \) the surface tension and \( E \) the Young modulus, while in the strong roughness
limit it becomes significantly large \([>2(\gamma E)^{1/2}]\) following the asymptotic behavior \( K \sim 2(\gamma E)^{1/2}
(\sigma \xi^H)^{1/2} \). © 1998 American Institute of Physics. [S0021-8979(98)07310-1]

I. INTRODUCTION

The statistical description of fracture surfaces in terms of
fractal theory has been a topic of intense research the past ten
years \(^1-3\) because of considerable fundamental and techno-
logical importance. A diverse variety of studies on very dif-
f erent materials (i.e., aluminium alloys, steels, titanium 6211,
rocks, intermetallics, glass, bakelite, porcelain, graphite, car-
bon surfaces, polymers, etc.), and with different techniques
[i.e., scanning electron microscopy, scanning tunneling mi-
croscopy, mechanical profilometry, electrochemistry, elec-
tron micrograph imaging, sectioning methods, etc.] revealed
that the corresponding static or roughness scaling exponent
was found in the range \( H \sim 0.6-1.0 \) \(^1-3\). All these experimen-
tal results in connection with theoretical ideas based on di-
rected polymer models supported enormously the idea that
fracture surfaces are commonly described in terms of self-
affine scaling with the most common roughness exponent
near the value \( H \sim 0.75 \). \(^2\)

Nevertheless, exponents close to the value \( H \sim 0.5 \)
(minimal energy surface) were also reported in cases which
can be considered very different. \(^3\) The existence of a univer-
sality class with \( H \sim 0.8 \) seemed to prevail when dynamical
effects (i.e., rapid crack propagation) play a significant role.\(^3,5,7\) Moreover, recent studies on fatigue fracture surfaces
of metallic alloys and stress corrosion fracture surfaces of
silicate glass by Daguier \(^5\) et al., revealed exponents close to
\( H \sim 0.5 \) at small length scales which cross over to the value
\( H \sim 0.78 \) at a length scale depends strongly on the material
and the crack velocity. However, despite the achieved con-
ensus up to now the universality of the roughness exponent
still remains controversial and under continuous investiga-
tion.\(^1-7\)

Furthermore, in the pioneering work by Mandelbrot \(^1\) et al., it was concluded that the fracture toughness \( K \) to be a
monotonic decreasing function of the fractal dimension \( D \) or
alternatively a monotonic increasing function of the rough-
ness exponent \( H \) since \( D = 2(3-H) \) (depending on the em-
bedding space dimensionality; two or three). \(^8\) Indeed, such a
result was rather surprising because one would expect a
rougher surface (smaller \( H \) at short length scales) to corre-
spond to a higher formation energy \(^8\) since larger surface area
will be created during fracture. This result gave rise to a
significant number of experimental investigations which
showed evidence for a correlation between fracture tough-
ness (or other material properties related to failure) and the
roughness exponent \( H \), as well as other studies reached dif-
derent conclusions. \(^2\) Nonetheless, because of the broad range
of materials and conditions used in fracture experiments, as
well as the uncertainties in the roughness measurements a
clear picture has not yet emerged.

A proper rewriting of the Griffith criterion for self-affine
cracks in brittle materials was proposed by Mosolov \(^7\) in or-
der to explain the increment of the fracture toughness with
the fractal dimension \( D \) and thus to resolve the controversy.
The calculations of the later approach were questioned by
Bouchaud \(^6\) et al., where by reapplication of the Griffith crite-
rian were shown that the critical fracture toughness \( K \) to be
constant for a typical surface height \( z \) (outside the fractal
regime) smaller than the in-plane roughness correlation
length \( \xi \), while in the opposite case \((z > \xi)\) to scale as \( K \sim (z/\xi)^{1/2} \). \(^6\) However, the previous qualitative result takes
into account only the long wavelength morphology charac-
teristics \((z, \xi)\), and neglects any dependence of the critical
toughness on finer roughness details at short wavelengths
\((< \xi)\) as described by the roughness exponent \( H \).

Therefore, further quantitative estimations of critical
fracture properties which will take into account all the char-
acteristic roughness components are in order. The latter will
be performed in terms of simple analytic surface models,
which however obey correctly the self-affine scaling hypoth-
esis, and allow quantitative derivation in a closed form of
important fracture and surface properties.

II. FRACTURE THEORY (ELASTIC AND SURFACE
ENERGY)

For simplicity we consider a sample of brittle material
with width \( W \) under a uniaxial tension, where crack propa-
gation occurs in mode I (perpendicular to the direction of the applied tension).\textsuperscript{5,7,9} According to the Griffith criterion,\textsuperscript{9} the critical value of the stress field at which crack propagation commences is determined by equating the elastic energy \( \Delta U_e \) due to crack propagation with the energy \( \Delta U_s \) required to create the two free surfaces in the material. Thus, one can obtain the critical value of the stress-intensity factor \( K \) below which the crack is unable to progress since the elastic energy is not sufficient to compensate for the creation of the two free surfaces.

Although a precise description of the evolution of surface fracture needs the use of dynamical equations with the appropriate geometric considerations, the Griffith criterion for brittle materials can provide a reasonable estimation of critical fracture properties for the simple case under consideration.\textsuperscript{6,7} It is very likely that different brittle materials show differences in terms of generation of a failure surface (due to dependence on material properties) that will be manifested by different surface fracture roughness parameters\textsuperscript{8} and critical properties (e.g., toughness). The latter can be correlated to the associated surface morphology in a simple manner by a proper application of the Griffith criterion.\textsuperscript{7}

In the following we assume the simple case of a self-affine fractal crack which looks as a one-dimensional straight line cut at macroscopic length scales, while in mesoscales and/or nanoscales as a rough fractal curve with dimension \( 1 < D < 2 \) because we consider for simplicity a two-dimensional problem. The stress field is assumed singular in the vicinity of the crack tip such that \( S(x) = K x^{-c} \) with \( K \) the stress intensity factor (fracture toughness), and \( x \) the distance ahead of the crack front. Since \( S^2/2E \) is the elastic energy per unit volume (with \( E \) the Young modulus), we can calculate the elastic energy \( \Delta U_e \) by considering the fact that the stress field is relaxed on length scales \( x < R \) and is unperturbed on larger scales \( (x > R) \). Thus, we obtain

\[
\Delta U_e \equiv (W/2E) \int_{r_0}^{R} S^2(x) \, dx
\]

\[
= [K^2/2E(-2c+2)] W R^{1-2c} - R^{-2c+2},
\]

(2.1)

where \( r_0 \) is a microscopic cutoff below which the stress field saturates (e.g., plastic zone size).

For a regular (flat) fracture path of length \( R \), the elastic energy is given by \( \Delta U_s \approx 2 \gamma WR \) with \( \gamma \) the surface tension. If the fracture surface is irregular and characterized by a random (single valued) fluctuation height \( z(x) \) along the horizontal axis of the crack, the energy required to create the two surfaces is given by

\[
\Delta U_s \approx 2 \gamma W \int_{a_0}^{R} \left( 1 + (dz/dx)^2 \right)^{1/2} \, dx.
\]

(2.2)

For a surface of small or large local surface slope \( |dz/dx| \), we obtain, respectively, after ensemble average over possible roughness realizations

\[
(\langle dz/dx \rangle \ll 1)
\]

\[
\langle |z(k)|^2 \rangle = \frac{A}{(2\pi)^2} \frac{\sigma^2 \xi}{(1 + a|k|\xi)^{1+2H}},
\]

(3.1)

where \( A \) is the macroscopic linear size of the system, and \( k_\eta = \pi / a_0 \). The normalization condition \( \int_{-k_\eta}^{k_\eta} \langle |z(k)|^2 \rangle \, dk = \sigma^2 \) yields the constant \( a \); \( a = (1/H)[1 - (1 + ak_\eta \xi)^{-2H}] \) if \( 0 < H < 1 \), and \( a = 2 \ln(1 + ak_\eta \xi) \) if \( H = 0 \).

In order to estimate the surface energy from Eq. (2.3), the rms local surface slope \( \rho \equiv \langle (dz/dx)^2 \rangle^{1/2} \) should be determined. By considering translation invariant surfaces \( \langle z(k)z(k') \rangle = [2(\pi)^2/4\pi^2 A] \delta(k + k') \langle |z(k)|^2 \rangle \), Fourier transforming and ensemble averaging over possible roughness realizations yields (see the Appendix)\textsuperscript{15}

\[
\rho(R) = \left[ 2(\pi)^2/4\pi^2 A \right] \int_{k_R}^{k_\eta} k^2 \langle |z(k)|^2 \rangle \, dk \right]^{1/2}
\]

(3.2)

with \( k_R = 2\pi/R \), and \( \rho(R) \ll \rho \) with \( \rho \) the local slope at \( R \gg \xi \). Substitution of Eq. (3.1) in Eq. (3.2) yields
IV. CRITICAL FRACTURE TOUGHNESS

Initially, we will estimate the elastic energy $\Delta U_s$ based on the knowledge of the rms local slope $\rho(R)$ given by Eq. (3.3). Assuming the height fluctuation $z(x)$ to be a Gaussian variable, we can obtain from Eq. (2.3) in the weak roughness limit the surface energy $\Delta U_s$ for a crack length $R$ (Appendix, Eqs. (A.1)–(A.2)). However, in the strong roughness limit, the inequality $\langle |d^2z/dx^2| \rangle \approx \langle |d^2z/dx^2|^2 \rangle^{1/2}$ yields an upper bound for the surface energy since $\int |d^2z/dx^2| dx \approx \int |d^2z/dx^2|^2 dx$. Thus, in both cases we obtain

$$\Delta U_s(R) = \begin{cases} 2\gamma WR \left(1 + (1/2)\rho(R)^2 - (3/8)\rho(R)^4 \ldots\right) & (\rho < 1), \\ 2\gamma WR \rho(R) & (\rho > 1). \end{cases}$$

In the following we will examine the behavior of the fracture toughness $K$ as a function of the roughness parameters $\sigma$, $\xi$, and $H$. At the onset of fracture, the critical fracture toughness $K$ will be obtained from the surface and elastic energies given by Eqs. (2.1)–(4.1) based on the Griffith criterion ($\Delta U_s = \Delta U_c$) for crack lengths $R$ significantly larger than the roughness correlation $\xi$ in order that the emerging surface morphology to display fully its self-affine nature determined from the parameters $\sigma$, $\xi$ and $H$. Finally, we will consider for simplicity the same lower cutoffs; $r_0 \approx a_0$.

Therefore, for $R \gg r_0$ Eq. (2.1) yields $\Delta U_c = [K^2/2E(-2c+2)]YR^{-2c+2}$ which in combination with Eq. (4.1) gives for large cracks ($R \gg \xi$) the stress field classical exponent $c \approx 0.5^9$ and the fracture toughness

$$K \equiv \begin{cases} 2(\gamma E)^{1/2} \left(1 + (1/2)\rho^2 - (3/8)\rho^4 \ldots\right)^{1/2} & (\rho < 1), \\ 2(\gamma E)^{1/2} \rho^{1/2} & (\rho > 1). \end{cases}$$

As Fig. (2) shows in the weak roughness limit, increment of the roughness exponent $H$ leads to decrement of the material critical toughness. For large roughness exponents $H \sim (-1)$ and large correlation lengths or small long wavelength ratios $\sigma/\xi$ for fixed $\sigma$ (surface smoothing), the critical toughness approaches asymptotically the classical value $K = 2(\gamma E)^{1/2}$ derived for planar fractured surfaces.9 Alternatively, this is depicted in the inset which shows $K$ vs $\sigma/\xi$. From both schematics we can conclude that in the weak roughness limit ($\rho < 1$) the critical toughness $K$ is more sensitive to variations of the roughness exponent $H$ rather than the long wavelength ratio $\sigma/\xi$.

In Fig. 3, we display simultaneously the weak roughness limit with the upper bound strong roughness limit21 of $K$ as a function of the long wavelength ratio $\sigma/\xi$ for two consecutive roughness exponents $H$ (in the range observed in fracture studies). In both schematics, there is a discontinuity of $K$ as function of $\sigma/\xi$ which signifies the cross over from the weak to the strong roughness limit regime. As the roughness exponent $H$ increases, even slightly, the cross over occurs at significantly larger ratios $\sigma/\xi$. The critical fracture toughness in the strong roughness limit ($\rho > 1$)21 can be significantly larger (depending on the roughness parameters) than that of a regular crack $\sim 2(\gamma E)^{1/2}$. This occurs mainly at large wavelength ratios $\sigma/\xi \sim 0.1$, and small roughness exponents $H \approx 0.5$.
The latter behavior is in agreement with the fact that as $H$ becomes smaller, the number of surface crevices increases$^{16}$ exposing therefore larger area which corresponds effectively to higher surface energies $\Delta U_j$. Alternatively, the full effect of the roughness exponent $H$ on the critical fracture toughness is depicted in Fig. (4), where we plot simultaneously the weak roughness limit with the strong roughness limit of $K$ vs $H$. The discontinuity of $K$ as function of $H$, which signifies the cross-over from the strong to weak roughness limit regime, occurs at lower roughness exponents as $\alpha/\xi$ decreases. Finally, if we compare Figs. 3 and 4 we can infer that the roughness exponent $H$ has the dominant effect on the critical fracture toughness rather than the long wavelength ratio $\alpha/\xi$.

Since $\rho^{=}\left\{1/(1-H)^{1/2}a_0^{1-H}a^H+1/2\right\}(\alpha/\xi^H)$ for $R\gg\xi$ and $\xi\gg a_0$, we obtain in the strong roughness limit from Eq. (4.2) the asymptotic behavior of the critical fracture toughness upper bound

$$K\approx2(\gamma E)^{1/2}\left\{1/(1-H)^{1/2}a_0^{1-H}a^H+1/2\right\}^{1/2}(\alpha/\xi^H)^{1/2},$$

(4.3)

which describes mainly the steep change of $K$ in Figs. 3 and 4 in the regime $K\gg2(\gamma E)^{1/2}$. Equation (4.3) shows that the critical fracture toughness scales as $K\sim(\alpha/\xi^H)^{1/2}$, which compares virtually to the scaling behavior $K\sim(z/\xi)^{1/2}$ derived in earlier studies by Bouchaud et al. $^6$ Nevertheless, Eq. (4.3) indicates that the critical toughness does not depend only on the long wavelength roughness characteristics $(\alpha/\xi)$, but also keeps a pronounced signature of the short wavelength surface details described by the roughness exponent $H$. By contrast, in the weak roughness limit, the surface irregularities only contribute additional terms to the fracture toughness of a flat crack of the order of $O(\alpha^2/\xi^{2H})$;

$$K\approx2(\gamma E)^{1/2}\left\{1+V(\alpha/\xi^{2H})+\cdots\right\}^{1/4}[1/(1-H)^{1/2}a_0^{1-H}a^H+1/2].$$

Several experimental studies in the past have shown the existence of a correlation between the fracture toughness and the fractal dimension of the emerging fractured surface.$^2$ Lung and Mu$^{22}$ applied the slit-island-method (introduced by Mandelbrot et al.$^1$) to measure the fractal dimension of fractured CrMnSiNi$_2$A steel specimens, and found a positive correlation between the fractal dimension $D$ and the logarithm of the fracture toughness; $D=\ln(K)$ (increment of $K$ corresponds to increment of $D$ or decrement of $H$ since $D=2-1/H$). Furthermore, it was shown that the measured fractal dimension is close to the intrinsic fractal dimension of the fractured metal surface when the used yardstick is small enough.$^{22}$ Finally, they explained that the origin of the negative correlation between fractal dimension and material toughness (decrement $K$ corresponds to increment of $D$) was that the yardstick used by previous authors for measuring $D$ was too large.$^{22}$

Comparison of our calculations with these experimental results is as follows. If in Eq. (4.3), which characterizes the strong roughness limit, substitute $D=2-H$ we obtain $D=[\ln(\xi)/(\xi/\alpha)]^{1/2}K+\alpha$ which indicates a positive correlation between fractal dimension $D$ and critical fracture toughness. Such a result compares qualitatively to the observed behavior in steel specimens,$^{22}$ $D=\ln(K)$ with a prefactor that is related directly to the roughness correlation length $\xi$. On the other hand, such a relation in former theoretical studies was not established.$^{6,7}$ Nevertheless, further experimental studies will be necessary in order for a full quantitative comparison between theory and experiment be established.

V. CONCLUSIONS

In conclusion, we convoluted information known from classical fracture theory (Griffith criterion) with that of analytic self-affine roughness models to describe fractured surfaces, in order to study morphology effects on rough crack properties. For large $(\gg\xi)$ crack sizes, the stress field singularity in the vicinity close to the crack tip involves the classical result $S(x)\sim x^{-1/2}$ both in the strong and weak roughness limit. The critical fracture toughness in the weak roughness limit remains close to the classical value $\sim2(\gamma E)^{1/2}$ for flat cracks. However, in the strong roughness
which represents all possible ways to group 2

Furthermore, in the strong roughness limit, the fracture toughness was found to evolve as a function of all the characteristic roughness parameters following the asymptotic behavior $K \sim (\sigma l H)^{1/2}$. Such a behavior compares to the behavior predicted in former fracture studies apart from the explicit dependence on the roughness exponent $H$. In both roughness limits, the actual fracture toughness was found to increase with decreasing roughness exponent $H$ or alternatively to be a monotonic increasing function of the local fractal dimension $D$ in agreement with former studies. We have thus shown the morphology of the fracture surface and the critical fracture toughness $K$ are closely related in a way that involves the complete set (by contrast to former studies) of self-affine roughness parameters $(H, \sigma, \xi)$ for large crack sizes ($\gg \xi$).

Finally, we should point out that for two-dimensional cracks similar results will hold qualitatively since the rms local slope still scales as $\rho \sim \sigma l H$. Moreover, despite the fact that we based our calculations on a simple analytic model, similar results are expected to hold for other correlation models which however satisfy the correct self-affine asymptotic limits.

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APPENDIX

If we assume the surface height $z(x)$ to be a Gaussian variable, then the average of any odd number of factors of $z(x)$ with the same or different arguments vanishes, whereas the average of the product of an even number is given by the sum of the products of the averages of $z(x)$'s paired two-by-two in all possible ways. Thus, as was shown in earlier studies, we have for statistically stationary surfaces up to second order (translation invariance) $\langle (z(k)z(k')) \rangle = [(2\pi)^{2s} A(L) \delta(k+k')] \langle z(k) \rangle^2$

$$
\left( \int \frac{dz}{dx} \right)^{2n} = (-1)^n \int \prod_{j=1}^{2n} z(k_j)
\times \prod_{j=1}^{2n} \frac{2\pi}{k_j} e^{-i2\pi k_j} \prod_{j=1}^{2n} dk_j = P(n) [\rho(R)]^{2n}
$$

(A1)

with $\rho(R)$ given by Eq. (3.2), $P(1) = 1$, and $P(2) = 3$. Further concepts of statistics are needed to calculate $P(n>2)$ which represents all possible ways to group $2n - z(q)$ en-

semble averaged in pairs of two. Thus, in the weak roughness limit for a crack of length $R(\rho<1)$, the surface energy is given by the general form

$$
\Delta U_s(R) \approx 2\gamma WR \left[ 1 + \sum_{n=1}^{+\infty} \left\{ \left[ (1/2(1-1)\cdots(1-2n+1) / n! \right] \right\} \times P(n) [\rho(R)]^{2n}. \right.
$$

(A2)

16. J. Krim and G. Palasantzas, Int. J. Mod. Phys. B 9, 599 (1995). See Fig. 1 in this reference for the effect of decreasing roughness exponent $H$ (increasing number of surface crevices) on the self-affine surface morphology.
21. For a Gaussian random variable $F$ it can be shown that $(|F|)=[(2\pi)^{1/2}]$. The latter allows a precise relation of the strong roughness limit with the upper bound roughness limit to within a constant factor of $(2\pi)^{1/2}$. But $(|F|)=[(2\pi)^{1/2}]$. The latter allows a precise relation of the strong roughness limit with the upper bound roughness limit to within a constant factor of $(2\pi)^{1/2}$.