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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 σ , the correlation length ξ , 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 $-1/2$ in both the strong and weak roughness limit. In the latter limit, the fracture toughness K remains close to the classical value $K \approx 2(\gamma E)^{1/2}$ with γ 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 $K \approx 2(\gamma E)^{1/2} (\sigma/\xi^H)^{1/2}$. © 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 years¹⁻³ because of considerable fundamental and technological importance. A diverse variety of studies on very different materials (i.e., aluminium alloys, steels, titanium 6211, rocks, intermetallics, glass, bakelite, porcelain, graphite, carbon surfaces, polymers, etc.), and with different techniques [i.e., scanning electron microscopy, scanning tunneling microscopy, mechanical profilometry, electrochemistry, electron micrograph imaging, sectioning methods, etc.] revealed that the corresponding static or roughness scaling exponent was found in the range $H \approx 0.6-1.0$.¹⁻³ All these experimental results in connection with theoretical ideas based on directed 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 $H \approx 0.75$.²

Nevertheless, exponents close to the value $H \approx 0.5^4$ (minimal energy surface) were also reported in cases which can be considered very different.⁵ The existence of a universality class with $H \sim 0.8$ seemed to prevail when dynamical effects (i.e., rapid crack propagation) play a significant role.^{3,6,7} Moreover, recent studies on fatigue fracture surfaces of metallic alloys and stress corrosion fracture surfaces of silicate glass by Daguier *et al.*,⁵ revealed exponents close to $H \approx 0.5$ at small length scales which cross over to the value $H \approx 0.78$ at a length scale depends strongly on the material and the crack velocity. However, despite the achieved consensus up to now the universality of the roughness exponent still remains controversial and under continuous investigation.¹⁻⁷

Furthermore, in the pioneering work by Mandelbrot *et al.*¹ 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 roughness 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 correspond to a higher formation energy⁶ 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 toughness (or other material properties related to failure) and the roughness exponent H , as well as other studies reached different 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 Mosolov⁷ in order to explain the increment of the fracture toughness with the fractal dimension D ⁷ and thus to resolve the controversy. The calculations of the later approach were questioned by Bouchaud *et al.*⁶ where by reapplication of the Griffith criterion 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 ξ , 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 characteristics (z, ξ), 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 characteristic 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 hypothesis, 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-

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gation occurs in mode I (perpendicular to the direction of the applied tension).^{6,7,9} According to the Griffith criterion,⁹ the critical value of the stress field at which crack propagation commences is determined by equating the elastic energy ΔU_e due to crack propagation with the energy ΔU_s required to create the two free surfaces in the material. Thus, one can obtain the critical value of the stress-intensity factor K^6 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.^{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 parameters⁸ 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.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 $S(x) = Kx^{-c}$ 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 ΔU_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

$$\Delta U_e \cong (W/2E) \int_{r_0}^R S^2(x) dx = [K^2/2E(-2c+2)]W(R^{-2c+2} - r_0^{-2c+2}), \quad (2.1)$$

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 $\Delta U_s = 2\gamma WR$ with γ 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

$$\Delta U_s \cong 2\gamma W \int_{a_0}^R [1 + (dz/dx)^2]^{1/2} dx. \quad (2.2)$$

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

$$\Delta U_s \cong \begin{cases} 2\gamma W \int_{a_0}^R \{1 + \frac{1}{2} \langle (dz/dx)^2 \rangle - \frac{1}{8} \langle (dz/dx)^4 \rangle \dots\} dx, & (|dz/dx| \ll 1) \\ 2\gamma W \int_{a_0}^R \langle |dz/dx| \rangle dx, & (|dz/dx| \gg 1), \end{cases} \quad (2.3)$$

where a_0 is an atomic cutoff below which any continuum description ceases to exist. At the onset of fracture, for the simple case of a flat crack of length $R \gg r_0$, the Griffith criterion ($\Delta U_e \approx \Delta U_s$) yields the classical stress field exponent $c = 1/2$ and the material dependent critical fracture toughness $K \approx 2(\gamma E)^{1/2}$.⁹

III. SELF-AFFINE SURFACE ROUGHNESS

For self-affine fractal surfaces the height-height correlation function $C(x) = \langle z(x)z(0) \rangle$ has the scaling behavior $C(x) \approx \sigma^2 - Bx^{2H}$ if $x \ll \xi$, and $C(x) = 0$ if $x \gg \xi^8$ with $B(\approx \sigma^2/\xi^{2H})$ a constant. ξ the in-plane roughness correlation length, $\sigma = \langle z(x)^2 \rangle^{1/2}$ the saturated rms surface roughness, and H ($0 < H < 1$) the roughness exponent which characterizes the degree of surface irregularity at small length scales ($x \ll \xi$).^{8,10} For self-affine fractals the roughness spectrum $\langle |z(k)|^2 \rangle \propto \int C(x) e^{-ikx} dx^{11}$ has the scaling behavior $\langle |z(k)|^2 \rangle \sim k^{-1-2H}$ if $k \xi \gg 1$, and $\langle |z(k)|^2 \rangle \sim \text{const}$ if $k \xi \ll 1$.⁸ Such behavior is satisfied by the simple analytic model^{12,13}

$$\langle |z(k)|^2 \rangle = \frac{A}{(2\pi)^2} \frac{\sigma^2 \xi}{(1 + a|k|\xi)^{1+2H}}, \quad (3.1)$$

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

In order to estimate the surface energy from Eq. (2.3), the rms local surface slope $\rho = [\langle |dz/dx|^2 \rangle]^{1/2}$ ^{14,15} should be determined. By considering translation invariant surfaces $\langle z(k)z(k') \rangle = [(2\pi)^2/A] \delta(k+k') \langle |z(k)|^2 \rangle$, Fourier transforming and ensemble averaging over possible roughness realizations yields (see the Appendix)¹⁵

$$\rho(R) = \left\{ [2(2\pi)^2/A] \int_{k_R < k < k_c} k^2 \langle |z(k)|^2 \rangle dk \right\}^{1/2} \quad (3.2)$$

with $k_R = 2\pi/R$, and $\rho(R) \leq \rho$ with ρ the local slope at $R \gg \xi$. Substitution of Eq. (3.1) in Eq. (3.2) yields

FIG. 1. Schematics of $\rho(R)$ vs H for $\sigma=1$ nm, $\xi=30, 50$ nm, $a_0=0.3$ nm, and a crack length $R=200$ nm ($R \gg \xi$). The inset shows schematics of $\rho(R)$ vs R for $\sigma=1$ nm, $\xi=30$ nm, $a_0=0.3$ nm, and roughness exponent in the range $0.5 \leq H \leq 0.8$.

$$\rho(R) = \frac{\sigma}{\xi} \sqrt{2a^{-3}} [F(ak_c \xi, H) - F(ak_R \xi, H)]^{1/2}. \quad (3.3)$$

with $F(y, H) = \{[(1+y)^2/(2-2H)] - [(1+y)/2(1-2H)] - 1/2H\}(1+y)^{-2H}$. For large length scales $R \gg \xi$, Eq. (3.3) yields the asymptotic value of the rms local surface slope $\rho \approx [1/(1-H)^{1/2} a_0^{1-H} a^{H+1/2}] (\sigma/\xi^H)$ (since $\xi \gg a_0$). Figure 1 depicts the extreme sensitivity of the local slope on the roughness exponent H in comparison with the long wavelength surface ratio σ/ξ .^{16,17} The inset shows the rather weak dependence of the rms local slope on the lateral length scale R .¹⁶⁻²⁰

IV. CRITICAL FRACTURE TOUGHNESS

Initially, we will estimate the elastic energy ΔU_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 ΔU_s for a crack length R (Appendix, Eqs. (A.1)–(A.2)). However, in the strong roughness limit, the inequality $\langle |dz/dx| \rangle \leq \langle |dz/dx|^2 \rangle^{1/2}$ yields an upper bound for the surface energy since $\int \langle |dz/dx| \rangle dx \leq \int \langle |dz/dx|^2 \rangle^{1/2} dx$.¹⁸⁻²¹ Thus, in both cases we obtain

$$\Delta U_s(R) \equiv \begin{cases} 2\gamma WR \{1 + (1/2)\rho(R)^2 - (3/8)\rho(R)^4 \dots\} & (\rho < 1), \\ 2\gamma WR \rho(R) & (\rho > 1). \end{cases} \quad (4.1)$$

In the following we will examine the behavior of the fracture toughness K as a function of the roughness parameters σ , ξ , 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 ($\Delta U_e \approx \Delta U_s$) for crack lengths R significantly larger than the roughness correlation ξ in order that the emerging surface morphology to display fully its self-affine

FIG. 2. Schematics of K vs H ($c=0.5$) in the weak roughness limit for a crack length $R(=200) \gg \xi$, $a_0=0.3$ nm, $\sigma=1$ nm, and various correlation lengths $\xi=20$ –60 nm. The inset shows K vs σ/ξ for the same roughness limit.

nature determined from the parameters σ , ξ 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 $\Delta U_e \approx [K^2/2E(-2c+2)]YR^{-2c+2}$ 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

$$K \equiv \begin{cases} 2(\gamma E)^{1/2} \{1 + (1/2)\rho^2 - (3/8)\rho^4 \dots\}^{1/2} & (\rho < 1) \\ 2(\gamma E)^{1/2} \rho^{1/2} & (\rho > 1) \end{cases}. \quad (4.2)$$

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 (~ 1) and large correlation lengths or small long wavelength ratios σ/ξ for fixed σ (surface smoothing), the critical toughness approaches asymptotically the classical value $K \approx 2(\gamma E)^{1/2}$ derived for planar fractured surfaces.⁹ Alternatively, this is depicted in the inset which shows K vs σ/ξ . 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 σ/ξ .

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 σ/ξ 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 σ/ξ 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 σ/ξ . 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 $\sim 2(\gamma E)^{1/2}$.⁹ This occurs mainly at large wavelength ratios $\sigma/\xi \sim 0.1$, and small roughness exponents $H(\leq 0.5)$.

FIG. 3. Schematics of K vs σ/ξ ($c=0.5$) for both roughness limits, a crack length $R(=200) \gg \xi$, $a_0=0.3$ nm, $H=0.7$, and $\sigma=5$ nm. The inset shows similar schematic but for $H=0.8$.

The latter behavior is in agreement with the fact that as H becomes smaller, the number of surface crevices increases¹⁶ exposing therefore larger area which corresponds effectively to higher surface energies ΔU_s . 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 .²¹ 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 σ/ξ 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 σ/ξ .

Since $\rho \approx [1/(1-H)^{1/2} a_0^{1-H} a^{H+1/2}] (\sigma/\xi^H)$ 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

$$K \approx 2(\gamma E)^{1/2} [1/(1-H)^{1/2} a_0^{1-H} a^{H+1/2}]^{1/2} (\sigma/\xi^H)^{1/2}, \quad (4.3)$$

which describes mainly the steep change of K in Figs. 3 and 4 in the regime $K > 2(\gamma E)^{1/2}$. Equation (4.3) shows that the critical fracture toughness scales as $K \sim (\sigma/\xi^H)^{1/2}$ ²¹ 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 (σ/ξ), 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 $O(\sigma^2/\xi^{2H})$; $K \approx 2(\gamma E)^{1/2} \{1 + V(\sigma^2/\xi^{2H}) + \dots\}$ with $V \approx (1/4)[1/(1-H)^{1/2} a_0^{1-H} a^{H+1/2}]$.

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

FIG. 4. Schematics of K vs H ($c=0.5$) for both roughness limits, a crack length $R(=200) \gg \xi$, $a_0=0.3$ nm, $\xi=50$ nm, and rms amplitude $\sigma=5$ nm. The inset shows similar schematic but for $\xi=100$ nm.

Lung and Mu²² applied the slit-island-method (introduced by Mandelbrot *et al.*¹) to measure the fractal dimension of fractured CrMnSiNi₂A steel specimens, and found a positive correlation between the fractal dimension D and the logarithm of the fracture toughness; $D \sim \ln(K)$ (increment of K corresponds to increment of D or decrement of H since $D=2-H$). 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 $D \approx [2/\ln(\xi)] \ln(K) + A$ 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 $D \sim \ln(K)$ with a prefactor that is related directly to the roughness correlation length ξ . 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 $\sim 2(\gamma E)^{1/2}$ for flat cracks. However, in the strong roughness

limit, it is proportional to the square root of the local rms slope which alternatively leads to large values of $K[>2(\gamma E)^{1/2}]$.

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 $K \sim (\sigma/\xi^H)^{1/2}$. Such a behavior compares to the behavior predicted in former fracture studies⁶ 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.²² 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^{6,7}) of self-affine roughness parameters (H, σ, ξ) 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 $\rho \sim \sigma/\xi_H$.¹⁵ 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.¹⁷

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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.¹⁸ Thus, as was shown in earlier studies,¹⁹ we have for statistically stationary surfaces up to second order (translation invariance) $\langle z(k)z(k') \rangle = [(2\pi)^2/A] \delta(k+k') \langle |z(k)|^2 \rangle$

$$\left\langle \left(\frac{dz}{dx} \right)^{2n} \right\rangle = (-1)^n \int \left\langle \prod_{j=1}^{2n} z(k_j) \right\rangle \times \left(\prod_{j=1}^{2n} k_j \right) e^{-i(\sum_{j=1}^{2n} k_j)x} \prod_{j=1}^{2n} dk_j = P(n) [\rho(R)]^{2n} \quad (\text{A1})$$

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 $2n-z(q)$ s en-

semble averaged in pairs of two.²⁰ Thus, in the weak roughness limit for a crack of length $R(\rho < 1)$, the surface energy is given by the general form

$$\Delta U_s(R) \cong 2\gamma WR \left[1 + \sum_{n=1}^{+\infty} \{ [1/2(1/2-1) \cdots (1/2-n+1)]/n! \} \times P(n) [\rho(R)]^{2n} \right]. \quad (\text{A2})$$

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