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Correlating toughness and roughness in ductile fracture

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Three dimensional calculations of ductile crack growth under mode I plane strain, small scale yielding conditions are carried out using an elastic-viscoplastic constitutive relation for a progressively cavitating plastic solid with two populations of void nucleating second phase particles. Full field solutions are obtained for three dimensional material microstructures characterized by random distributions of void nucleating particles. Crack growth resistance curves and fracture surface roughness statistics are calculated using standard procedures. The range of void nucleating particle volume fractions considered give rise to values of toughness, $J_{IC}$, that vary by a factor of four. For all volume fractions considered, the computed fracture surfaces are self-affine over a size range of about two orders of magnitude with a roughness exponent of 0.54 ± 0.03. For small void nucleating particle volume fractions, the mean large particle spacing serves as a single dominant length scale. In this regime, the correlation length of the fracture surface corresponding to the cut-off of the self-affine behavior is found to be linearly related to $J_{IC}$ thus quantitatively correlating toughness and fracture surface roughness.

Thirty years ago, Mandelbrot and coworkers revealed the self-affine nature of fracture surfaces [1]. Their hope was to relate the roughness of fracture surfaces via the exponents characterizing their scale invariance properties to the material’s crack growth resistance. This hope has remained unfulfilled. Indeed, later studies showed that the value of the roughness exponent was not only independent of the material toughness but also of the material considered, as long as the failure mechanism remained the same [2, 3]. Indeed, the scaling exponent measured along the propagation direction was observed to take a value $\beta_{\text{brittle}} \approx 0.5$ rather independent of the considered material for brittle failure while another value around $\beta_{\text{damage}} \approx 0.6$ was observed for damage accompanying failure [4, 5].

The universality of fracture surface roughness exponents limits the applicability of quantitative fractography based on statistical analyses for the characterization of microscopic failure mechanisms and toughness. On the other hand, it has paved the way for a unified theoretical framework based on critical transition theory to describe the failure properties of disordered materials. By interpreting the onset of material failure as a dynamic phase transition, many aspects of the behavior of cracks in disordered materials has thus been rationalized, such as the intermittent dynamics of cracks [6, 7], their scale invariant roughness [8, 9], their average dynamics [10, 11] and their effective toughness [12, 13]. Most of these successes have been achieved in the context of brittle failure, but our understanding of the scaling properties of ductile fracture surfaces is still limited.

The process that governs the ductile fracture of structural materials at room temperature is one of nucleation, growth and coalescence of micron scale voids, and involves large plastic deformations. Quantitative models of crack growth by the progressive coalescence of voids with a crack have been available since the 1970s [14-17], and calculations have provided reasonable agreement with experimental toughness measurements [18]. However, only recently has the capability been developed to calculate sufficient amounts of three dimensional ductile crack growth in heterogeneous microstructures to obtain a statistical characterization of the predicted fracture surfaces [19, 20]. This enables us to explore the microscopic mechanisms governing the fracture surface roughness as well as the relation, if any, to a material’s crack growth resistance.

In this study, we capitalize on these new developments and show that the scaling properties of ductile cracks can correlate with the material’s toughness. However, the relation is not with the value of the roughness exponent, but with the cut-off length of the scale invariant regime. In particular, we show that the cut-off length scale of the self-affine behavior of ductile cracks can be quantitatively related to a measure of fracture toughness. This correlation is shown in our simulations by varying one parameter of the material microstructure resulting in a family of ductile materials with a broad range of toughness.

Model formulation – The connection between the roughness of ductile cracks and the material’s toughness is investigated through the finite element analysis of transient three dimensional boundary value problems. A mode I small scale yielding boundary value problem is analyzed with symmetry conditions corresponding to an overall plane strain constraint. Remote displacement boundary conditions corresponding to the quasi-static linear isotropic elastic mode I crack tip stress intensity factor $K_I$ are prescribed. A finite deformation continuum mechanics formulation for a progressively cavitating solid is
used. The constitutive framework is a modified Gurson constitutive relation for a progressively cavitating solid (often termed the GTN relation, see \[21\]) with slight material rate dependence and with the plastic flow potential \(\Phi\) given by

\[
\Phi = \frac{\sigma_e^2}{\sigma_s^2} + 2q_1f^* \cosh \left( \frac{3q_2\sigma_h}{2\sigma} \right) - 1 - (q_1f^*)^2 = 0 \tag{1}
\]

where \(\sigma_e\) is the Mises effective stress, \(\sigma_h\) is the hydrostatic stress (positive in tension), \(\sigma\) is the material flow strength, \(f^*\) is a measure of the void volume fraction and \(q_1 = 1.25\) and \(q_2 = 1.0\). A key feature of the constitutive relation is that the material’s stress carrying capacity increases due to strain and strain rate hardening, but eventually decreases due to the nucleation and growth of micro-voids, and can vanish leading to the creation of new free surface.

The second phase particles present in conventional structural metals are the primary source of internal cavitation at least at low temperatures. Hence we characterize the material microstructure by two populations of void nucleating second phase particles: (i) homogeneously distributed small particles and (ii) discretely modeled randomly distributed large particles. For homogeneously distributed small particles, a critical strain level following a normal distribution controlled void nucleation. Void nucleation from large particles in general depends on deformation and hydrostatic stress history. Hence, nucleations occur when \(\sigma + \sigma_h\) reaches a critical value taken here also from a normal distribution. Following this stress based criteria, the large particles nucleate voids at an early stage of the deformation history.

The large particles are randomly located, and the maximum stress based void nucleation criteria is applied in a sphere of radius \(r_0\) around their center. The elastic and plastic properties of the particles and the matrix material are identical. Only the void nucleation characteristics differ. A uniform \(208 \times 64 \times 10\) mesh of 20 node brick finite elements is used in front of the initial crack. The in-plane \((x-y)\) element dimension is denoted by \(e_x\), which serves as a normalization length. The size and spacing of the large particles introduce characteristic lengths into the formulation. The particles radius, \(r_0 = 1.5e_x\), is fixed and calculations are carried out for eight volume fractions, \(n\), of the large particles. For each large particle volume fraction, calculations were carried out for seven random spatial distributions. A more detailed description of the problem formulation with additional references is given in \[11, 22\].

**Toughness characterization** – The volume fraction of large particles is varied from \(n = 0.012\) to \(n = 0.19\), corresponding to mean large particle spacings of \(10.6e_x\) and \(4.21e_x\), respectively. Under plane strain conditions, the \(J\)-integral \[22\], a measure of the driving force for crack propagation, is related to the applied mode I stress intensity factor, \(K_I\), by

\[
J = K_I^2 \left( \frac{1 - \nu^2}{E} \right) \tag{2}
\]

where \(E = 70\) GPa, and \(\nu = 0.3\) are Young’s modulus and Poisson’s ratio, respectively. Figure \[1\] shows the variation of \(J_{IC}\), normalized by the reference flow strength \(\sigma_0 = 300\) MPa and \(e_x\), with large particle volume fraction \(n\). The error bars are calculated from realizations of large particle distributions having the same \(n\). The value of \(J_{IC}\) characterizes the crack growth resistance and is computed using a widely used ASTM standard procedure \[23\]. A power law \(J = C_1 \Delta a^{C_2}\) is used to fit the initial portion of the \(J-R\) curve (shown in the inset of Fig. \[4\] for two values of \(n\)) and the value of \(C_2\) is defined as the intersection of this curve with the line \(J = 2\sigma_0 (\Delta a - \Delta a_0)\), where we take \(\Delta a_0/e_x = 2\). Another choice in the value of \(\Delta a_0\) would change the value of \(J_{IC}\) but the dependence of \(J_{IC}\) on \(n\) would remain approximately the same up to some multiplicative constant. The increase in the value of \(J\) with the crack extension \(\Delta a\) seen in the inset of Fig. \[4\] is characteristic of ductile crack growth.

From dimensional considerations alone, prediction of the \(J(\Delta a)\) curve requires that the formulation contain a characteristic length. The value of \(J_{IC}\) increases by a factor of almost four as the volume fraction of large particles decreases or, equivalently, with an increasing mean particle spacing. Indeed, in the calculations here, the mean particle spacing serves as a microstructurally based characteristic length for the entire \(J(\Delta a)\) curve as well as for \(J_{IC}\).

**Fracture surface characterization** – For each value of large particle volume fraction, \(n\), fourteen statistically equiv-
shows a clear correlation of the volume fraction $n$ of the large particles. Inset: Snapshot of the porosity field for a material with $n = 0.048$ showing a propagating ductile crack. The white region corresponds to a porosity larger than the threshold value 0.1 used to define the fracture surface.

![Figure 2: Height-height correlation functions of the fracture surface showing the effect of the volume fraction $n$ of the large particles. Inset: Snapshot of the porosity field for a material with $n = 0.048$ showing a propagating ductile crack. The white region corresponds to a porosity larger than the threshold value 0.1 used to define the fracture surface.](image)

The roughness is characterized using the height-height correlation function defined as

$$\Delta h(\delta x) = \sqrt{\langle [h(x + \delta x, y) - h(x, y)]^2 \rangle_{x,y}}$$  \hspace{1cm} (3)$$

and computed on the statistically equivalent surfaces. We focus here on the correlations of height variations in the propagation direction $x$. The effect of the particle volume fraction $n$ on the fracture surface scaling is shown in Fig. 2. Regardless of the value of $n$, the correlation function follows a power law behavior at small scales and then saturates at a larger scale, indicating a self-affine behavior of the roughness up to some cut-off length $\xi$. The latter is defined at the absissa between the power-law fit of the self-affine regime and the plateau behavior at the larger scale. The first regime is characterized by the roughness exponent $\beta \simeq 0.54 \pm 0.03$ corresponding to the slope of a straight line fit in the logarithm representation of Fig. 2. This value is not affected by the large change in the particle spacing, as observed in the inset of Fig. 2, where the value of $\beta$ is shown as a function of the particle volume fraction $n$. This observation is in agreement with previous results obtained from similar simulations \[19, 20\], and captures rather well the universal self-affine nature of ductile fracture surfaces with $\beta \simeq 0.6$ observed experimentally \[21\]. As can be seen in Fig. 2, both the roughness amplitude in the self-affine regime, exemplified by the vertical shift of the correlation function, and the plateau level do vary with $n$. This dependence is reflected in the cut-off length scale $\xi$ that represents the upper bound of the self-affine domain. As shown in Fig. 2, $\xi$ decreases with increasing large particle volume fraction, i.e., with decreasing mean large particle spacing. Also, the analysis of the full statistics of the crack roughness obtained from this calculation and presented in Ref. \[20\] shows strong deviations from the Gaussian distribution, in agreement with experimental observations \[23\].

**Toughness/roughness relationship** – The variation of $\xi$ with $J_{IC}$ presented in Fig. 4 shows a clear correlation between a measure of the ductile fracture surface roughness, $\xi$, and a measure of the material’s resistance to crack growth, $J_{IC}$. For brittle solids, a relation between the critical stress intensity factor $K_{IC}$ and a cut-off length is discussed in Ref. \[26\]. The length $\xi$ can be interpreted as the typical size of the largest roughness features along the mean fracture plane. As a result, within the family of ductile solids investigated, with the exception of the two largest particle densities, the tougher the material, the rougher its fracture surface.

**Discussion** – To understand the $\xi$ versus $J_{IC}$ correlation, we first examine the mechanisms that set the length scale $\xi$. Previous experimental studies on glass and mortar fracture surfaces have reported two scaling regimes $\Delta h \sim \delta x^\beta$, with $\beta_{\text{damage}} \simeq 0.6$ at small length scales $\delta x < \xi$ and $\beta_{\text{brittle}} \simeq 0.5$ at larger length scales $\delta x > \xi$
shows the relation between toughness and roughness: Variance in terms of process zone size, or extension of the zone in the vicinity of the crack tip, both the fracture surface roughness and the overall crack growth resistance would be dominated by the single microstructural length scale \( \ell_0 \), leading to a linear relation between \( \xi \) and \( J_{IC}/\sigma_0 \) as seen in Fig. 4. In addition, since the plastic zone size scales with \( J/\sigma_0 \), \( \xi \) is also linearly related to the plastic zone size.

The idealized calculation of Ref. [16] introduces the dimensionless parameter \( C = J_{IC}/(\sigma_0 \ell_0) \) that reveals which of these ductile failure mechanisms dominates. In our calculations, \( C \approx 1.0 \) for \( n = 0.012 \) and saturates to a value of \( C \approx 0.68 \) for \( n \geq 0.071 \) (a saturation in the value of \( J_{IC} \) and \( \xi \) for \( n \geq 0.071 \) can also be seen in Figs. 4 and 3). A rough comparison with the values of \( C \) obtained in Ref. [16] suggests that the void by void crack growth is the dominant mechanism for \( n < 0.071 \), in agreement with the scenario proposed previously to explain the linear relation between \( \xi \) and \( J_{IC}/(\sigma_0 \ell_0) \). For \( n \geq 0.071 \), the value of \( C \) is consistent with another competing mechanism where crack growth is dominated by multiple voids (or more generally defects) interaction, accounting for the deviation from a linear relation seen at smaller values of \( \xi \) in Fig. 4 for greater volume fractions of large particles (or smaller mean particle spacings). A more detailed analysis of these competing mechanisms is underway. When multiple defect interactions become more prevalent, the mean particle spacing \( \ell_0 \) is no longer the only relevant roughness length scale and the linear relation between \( \xi \) and \( J_{IC}/(\sigma_0 \ell_0) \) breaks down. Conclusion—Our calculations show that: (i) with a random distribution of void nucleating particles and fixed material properties, the mean particle spacing is the dominant length scale; (ii) the roughness correlation length \( \xi \), corresponding to the cut-off of the self-affine behavior, reflects this length scale; (iii) \( \xi \) is linearly related to \( J_{IC} \) as long as one length scale characterizes the microscale fracture process. These results provide an important step toward fulfilling the hope that the statistical characteri-
zation of ductile fracture surface roughness may be used for a post-mortem estimate of fracture toughness.

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[1] B. B. Mandelbrot, D. E. Passoja, and A. J. Paullay, Nature 308, 721 (1984).
[2] E. Bouchaud, G. Lapasset, and J. Planès, Europhys. Lett. 13, 73 (1990).
[3] K. J. Máloý, A. Hansen, E. L. Hinrichsen, and S. Roux, Phys. Rev. Lett. 68, 213 (1992).
[4] D. Bonamy and E. Bouchaud, Phys. Rep. 498, 1 (2011).
[5] L. Ponson, H. Auradou, P. Vié, and J. P. Hulin, Phys. Rev. Lett. 97, 125501 (2006).
[6] K. J. Máloý, S. Santucci, J. Schmittbuhl, and R. Toussaint, Phys. Rev. Lett. 96, 045501 (2006).
[7] D. Bonamy, S. Santucci, and L. Ponson, Phys. Rev. Lett. 101, 045501 (2008).
[8] J. Schmittbuhl, S. Roux, J. P. Vilotte, and K. J. Máloý, Phys. Rev. Lett. 74, 1787 (1995).
[9] S. Santucci, M. Grob, R. Toussaint, J. Schmittbuhl, A. Hansen, and K. J. Máloý, Eur. Phys. J. 92, 44001 (2010).
[10] J. Koivisto, J. Rosti, and M. J. Alava, Phys. Rev. Lett. 99, 145504 (2007).
[11] L. Ponson, Phys. Rev. Lett. 103, 055501 (2009).
[12] V. Demery, A. Rosso, and L. Ponson, Cond-mat/ArXiv:1212.1551 (2013).
[13] S. Patinet, D. Vandembroucq, and S. Roux, Phys. Rev. Lett. 110, 165507 (2013).
[14] J. Rice and A. Johnson, Inelastic Behavior of Solids (eds. M. F. Kanninen, et al.) pp. 641–672 (1970).
[15] N. Aravas and R. M. McMeeking, J. Mech. Phys. Solids 33, 25 (1985).
[16] V. Tvergaard and J. Hutchinson, Int. J. Solids Struct. 39, 3581 (2002).
[17] I. Afek, E. Bouchbinder, E. Katzav, Mathiesen, and I. Procaccia, Phys. Rev. E 71, 066127 (2005).
[18] R. Becker, A. Needleman, S. Suresh, V. Tvergaard, and A. Vasudevan, Acta metall. 37, 99 (1989).
[19] A. Needleman, V. Tvergaard, and E. Bouchaud, J. Appl. Mech. 79, 031015 (2012).
[20] L. Ponson, Y. Cao, E. Bouchaud, V. Tvergaard, and A. Needleman, Int. J. Fract. p. 1 (DOI 10.1007/s10704-013-9846-z).
[21] V. Tvergaard, Adv. Appl. Mech. 27, 83 (1990).
[22] J. Rice, J. Appl. Mech. 35, 379 (1968).
[23] ASTM E1820-11 (Standard Test Method for Measurement of Fracture Toughness, ASTM International, 2011).
[24] L. Ponson, D. Bonamy, and E. Bouchaud, Phys. Rev. Lett. 96, 035506 (2006).
[25] S. Vernède, J.-P. Bouchaud, Y. Cao, and L. Ponson (submitted for publication).
[26] E. Bouchaud and J.-P. Bouchaud, Phys. Rev. B 50, 17752 (1994).
[27] D. Bonamy, L. Ponson, S. Prades, E. Bouchaud, and C. Guillot, Phys. Rev. Lett. 97, 135504 (2006).
[28] S. Morel, D. Bonamy, L. Ponson, and E. Bouchaud, Phys. Rev. E 78, 016112 (2008).
[29] D. Dalmas, A. Lelarge, and D. Vandembroucq, Phys. Rev. Lett. 101, 255501 (2008).
[30] S. Ramanathan, D. Ertas, and D. S. Fisher, Phys. Rev. Lett. 79, 873 (1997).