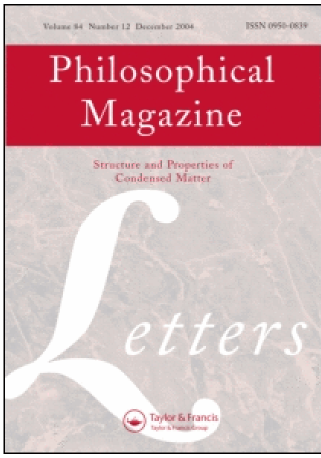

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A multiscale Griffith criterion

S. Li [a]
[a] Department of Civil and Environmental Engineering, University of California, Berkeley, CA94720, USA

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A multiscale Griffith criterion

S. LI*

Department of Civil and Environmental Engineering,
University of California, Berkeley, CA94720, USA

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In this letter, a compatibility-momentum tensor is proposed based on the strain compatibility condition of continuum mechanics. By rescaling the compatibility-momentum tensor, we construct a so-called multiscale energy-momentum tensor and the corresponding L-integral, which is path-independent if the interior region of the integration contour is dislocation-free. By applying the invariant L-integral to the field of a mode III elastoplastic crack under small-scale yielding condition, we derive a multiscale criterion for macroscopically brittle fractures.

1. Introduction

Fracture is a multiscale phenomenon in condensed matter physics, e.g. [1]. The first milestone of fracture mechanics is Griffith's energy criterion for brittle crack growth [2], which has been extensively used in solving linear elastic fracture mechanics (LEFM) problems. Due to the emergence of nanotechnology, the size and scaling effects of fracture on material strength have become central issues for nanomaterials and their modelling. Significant discrepancies in the critical stress predictions have been reported in the literature between the classical Griffith criterion and the results obtained from atomistic simulations, e.g. [3, 4]. These discrepancies have been attributed to several factors: lattice trapping, twinning, recrystallization, grain boundary migrations, and in general dislocation motions.

In this letter, a multiscale energy criterion is proposed to characterize *macroscopically brittle fracture*, which takes into account contributions due to both surface separation and geometrically necessary dislocation (GND) release during crack growth at small scale. In passing, we note that the letter refrains from discussions of ductile fracture, which may need different approaches, e.g. [5].

*Email: shaofan@berkeley.edu

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2. Multiscale energy-momentum tensor

The idea and procedure of forming a multiscale energy–momentum tensor are as follows. Assume that the total infinitesimal displacement field of a deformed solid can be decomposed into multiscale components,

$$\boldsymbol{u}(\mathbf{X}) = \bar{\boldsymbol{u}}(\mathbf{X}) + \boldsymbol{u}'(\mathbf{X}) \tag{1}$$

where $\bar{\mathbf{u}}$ is the coarse (macro-) scale displacement field, which may be viewed as a mean field; while $\mathbf{u}'$ is the fine (micro-) scale displacement field, which can be affected by the presence or fluctuation of defect distributions. Moreover, we assume that the fine-scale defect distribution is localized so after homogenization the coarse-scale deformation field is simply a linear elastic solid. The total strain field can thus decompose to

$$\boldsymbol{\epsilon} = \bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}' = \bar{\boldsymbol{\epsilon}} + \boldsymbol{\epsilon}^{e\,\prime} + \boldsymbol{\epsilon}^{p\prime} = \boldsymbol{\epsilon}^{e} + \boldsymbol{\epsilon}^{p} \tag{2}$$

Where $\bar{\epsilon} = \bar{\epsilon}^e = Sym(\nabla \otimes \bar{\mathrm{u}})$, and both ϵ'_e and ϵ'_p are incompatible elastic and plastic strains. Note that $\epsilon^e = \bar{\epsilon}^e + \epsilon^{e'}$ and $\varepsilon' = \varepsilon^{p\prime}$. We now propose the following multiscale free-energy density,

$$W^m(\bar{\boldsymbol{u}},\boldsymbol{\epsilon}^{e'}) = W^c(\bar{\boldsymbol{u}}) + W^f(\boldsymbol{\epsilon}^{e'}) \tag{3}$$

where the coarse-scale strain energy density is

$$W^c = \frac{1}{2}\bar{\boldsymbol{\epsilon}}^e : \bar{\mathbf{C}} : \bar{\boldsymbol{\epsilon}}^e \tag{4}$$

and $\bar{\mathbf{C}}$ is the coarse-scale elastic stiffness tensor. The fine-scale free-energy density is

$$W^f(\boldsymbol{\epsilon}^{e'}) := \frac{\mu\ell^2}{2}\boldsymbol{\zeta} : \boldsymbol{\zeta}^T = \frac{\mu\ell^2}{2}\zeta_{ij}\zeta_{ji}, \tag{5}$$

where $\zeta_{ij} := e_{ik\ell}\epsilon^e_{\ell j,k} = e_{ik\ell}\epsilon^{e'}_{\ell j,k}$ is the curl of the elastic strain, $e_{ik\ell}$ is the permutation symbol, μ is the fine-scale elastic shear modulus, and ℓ is a length-scale or the gauge length-scale [6], below which the coarse-scale observer cannot see. The factor $\mu\ell^2$ in Equation 5 will make the physical unit of the term $W^f(\boldsymbol{\epsilon}^{e\prime})$ as the unit of energy, density, i.e. energy per unit volume.

We note that similar types of free-energy densities have been proposed by others, e.g. [6–8]. In particular, Kleinert specifically collect a similar form of (5) 'the defect gauge field', and he labelled the penalty term as the contribution of 'the rotational stiffness'. However, the main difference between the current approach and Kleinert's approach is that we regard (3) as a multiscale free-energy density, in which $\bar{\boldsymbol{u}}$ and $\boldsymbol{\epsilon}^{e\prime}$ are independent, whereas in the formulations of Kleinert and others, it is an elastic free-energy of a second-order strain gradient theory where the displacement field and the plastic strain field are coupled. This leads to the divergence of two different approaches:

(1) We view equation (3) as a general decomposition that does not depend on specific inelastic microscale constitutive relations. One can find the fine-scale free-energy density, $W^f(\boldsymbol{\epsilon}^e)$, as long as the continuum measure of the GND

distribution is given in terms of ϵ^e or ϵ^p regardless of which constitutive relations it comes from; whereas

(2) Kleinert and others used the coupled higher order strain energy density to derive or to constrain microscale plasticity constitutive relations. That is, their free-energy density, which is not a multiscale formulation, affects the plasticity constitutive relations at microscales.

The essence of the proposed multiscale theory is that by assuming the fine-scale dislocation distribution is small and in steady state, the defect distribution can be given a priori without affecting the coarse-scale (macro-) constitutive relation. Hence we can then extrapolate a universal form of multiscale elastic free-energy from the global (coarse-scale) deformation as well as the (fine-scale) defect distribution, whereas in the strain gradient theory or the dislocation gauge theory one has a higher order elastic free-energy density first, and then tries to derive a microscale constitutive relation, hoping eventually to solve for dislocation or defect distributions under the particular constitutive relation. A detailed discussion on ramifications of these two different approaches and their thermodynamic consequences will be presented in a full-length paper [9].

Through a rigorous variational approach [9], we have found that the defect potential (5) is variationally meaningful. That is, the first variation of the potential yields a stationary condition that is the Saint-Venant compatibility condition [10],

$$\delta \int_V W^f(\epsilon^e)dV = 0 \;\Rightarrow\; e_{irk}e_{js\ell}\epsilon^e_{rs,\ell k} = 0, \tag{6}$$

if the domain of interest is compatible or defect-free. Therefore the physical meaning of the potential (5) is a quantity that is proportional to the free energy of the defect, specifically the dislocation distribution.

By applying Noether's theorem, one can find a compatibility-momentum tensor due to translation symmetry of the potential (5),

$$S^f_{k\alpha} = W^f\delta_{k\alpha} - \mu\ell^2 e_{mki}\zeta_{jm}\epsilon^e_{ij,\alpha}. \tag{7}$$

We then construct a multiscale energy–momentum tensor by combining the coarse-scale energy–momentum tensor and the fine-scale energy momentum tensor, i.e. the compatibility-momentum tensor,

$$S^m_{k\alpha} = S^c_{k\alpha} + S^f_{k\alpha} \tag{8}$$

in which

$$S^c_{k\alpha} = W^c\delta_{k\alpha} - \bar{u}_{\ell,\alpha}\bar{\sigma}_{k\ell} \tag{9}$$

is Eshelby's energy–momentum tensor [11, 12], $\bar{\sigma}_{ij}$ is the coarse-scale Cauchy stress, $\bar{u}_\ell$ is the coarse-scale displacement field, and $\delta_{k\alpha}$ is the Kronecker delta. Note that the subscript, 'α' denotes the spatial derivative.

We argue that the stress measure is a macro quantity, and the strain measure can be a micro quantity. Accordingly, the multiscale energy–momentum tensor, $S^m_{k\alpha}$, has two scale components: a coarse part to describe macroscale brittle cleavage surface separation and a fine-scale part to describe dislocation motions.

By virtue of the equilibrium equation $\sigma_{ij,i} = 0$, one can show that Eshelby's energy–momentum tensor obeys $S^c_{k\alpha,k} = 0$. Similarly via the compatibility condition (6), it is easy to show that $S^f_{k\alpha,k} = 0$, if there is no inelastic deformation in the solid. We may call $S^f_{k\alpha}$ the compatibility-momentum tensor, because it is derived based on the symmetry condition of compatibility conditions [13]. Conceptually, configurational compatibility forms a duality pair with configurational force [14].

We can then calculate the multiscale configurational force,

$$\mathcal{L}_\alpha = \bar{J}_\alpha + L_\alpha \tag{10}$$

where the coarse-scale configurational force is the J-integral [15],

$$\bar{J}_\alpha := \oint_{\Gamma_c} S^c_{k\alpha} n_k dS \tag{11}$$

where n_k is the surface normal of Γ_c, and the fine-scale configurational force is the L-integral,

$$L_\alpha := \oint_{\Gamma_f} S^f_{k\alpha} n_k dS \tag{12}$$

which is a measure of configurational compatibility. Since both integrals are path independent, their linear combination is also path independent. In the rest of this letter, we denote the first component of $\mathcal{L}_\alpha$ as the multiscale L-integral, i.e. $L^m = \mathcal{L}_1$, which may represent the driving force for a macroscopically brittle crack moving in the x_1 direction.

As an example, we now calculate the L^m-integral for a mode-III steady-state elastoplastic crack growth problem whose solution is given by Hult and McClintock (HM) [16] which is under the assumption of small-scale yielding. The integration contour, Γ_c, can be taken arbitrarily over the coarse-scale field as long as it contains the crack tip, whereas the fine-scale integration contour, Γ_f, is taken as the boundary of the plastic region, or process zone, i.e. S (see figure 1). In the calculation, we choose the contour for the coarse-scale J-integral to be slightly (infinitesimally)

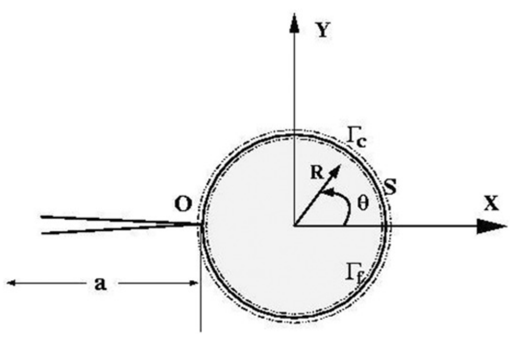

Figure 1. Schematic illustration of a macroscopically brittle crack.

larger than S, i.e. $\Gamma_c = S^+$ (since it cannot see the fine scale), whereas the contour for the fine-scale L-integral is slightly (infinitesimally) smaller than S, i.e. $\Gamma_f = S$. Suppose the crack length is denoted as a, and the remote stress is τ_∞. The multiscale driving force is

$$L^m = \left(\frac{\pi\tau_\infty^2}{2\mu}\right)a + \left(\frac{3l^2\pi\tau_0^4}{8\mu\tau_\infty^2}\right)\frac{1}{a}. \tag{13}$$

where we neglect the difference between the macro shear modulus and the micro shear modulus, i.e. $\bar{\mu} = \mu$.

To investigate the behaviour of the multiscale driving force, we perform a stability analysis of the equilibrium. For a macroscopically brittle fracture, we may assume a constant fracture resistance, i.e. $R = \text{const.}$ and $\partial R/\partial a = 0$. Thus $\partial L^m/\partial a < 0$ implies stable crack growth, or simply stability. The minimum may be found via the stationary condition,

$$\left.\frac{\partial L^m}{\partial a}\right|_{\tau_\infty} = \left(\frac{\pi\tau_\infty^2}{2\mu}\right) - \left(\frac{3l^2\pi\tau_0^4}{8\mu\tau_\infty^2}\right)\frac{1}{a^2} = 0. \tag{14}$$

Under load control, the minimum driving force to advance a crack and the stability point are given as

$$L^m_{\min} = \frac{\pi\tau_\infty^2 a_{\min}}{\mu}, \quad \text{and} \quad a_{\min} = \frac{\sqrt{3}}{2}\left(\frac{\tau_0}{\tau_\infty}\right)^2 \ell. \tag{15}$$

The physical meaning of $a_{\min}$ is the crack length at instability.

We note that these findings indicate that an incompatible field will yield a minimum driving force. In addition, incompatibility enables stable crack growth during load control. To frame the discussion with respect to the applied loading, we find that the far-field stress at instability is

$$\tau_{\infty,\min} = \left(\frac{3}{4}\right)^{1/4}\sqrt{\frac{\ell}{a_{\min}}}\tau_0. \tag{16}$$

By assuming that $a_{\min} \sim \mathcal{O}(\ell)$, the critical stress for brittle fracture at small scale may be estimated as $\tau_\infty^{cr} \sim 0.75\tau_0$ where τ_0 may be viewed as the theoretical strength or the cohesive strength of the material. The driving force can be normalized by $L^m_{\min}$,

$$\frac{L^m}{L^m_{\min}} = \frac{1}{2}\left(\frac{a}{a_{\min}} + \frac{1}{a/a_{\min}}\right). \tag{17}$$

In figure 2, we plot the multiscale driving force with different normalization against the normalized crack length. It can be seen from figure 2 that there is a well located minimum at $a_{\min}$. This suggests that the driving force for crack growth at small scale cannot be zero, even if the crack length, a, approaches zero. This is because the total energy release has two sources: (1) the strain energy release due to the surface separation at macroscale, and (2) the misfit energy release, as a form of strain-gradient energy release, due to the change of the defect potential. The change of the defect potential can be interpreted as due to the GND absorption or release, deformation twinning, or other incompatible strain field releases. At the small scale,

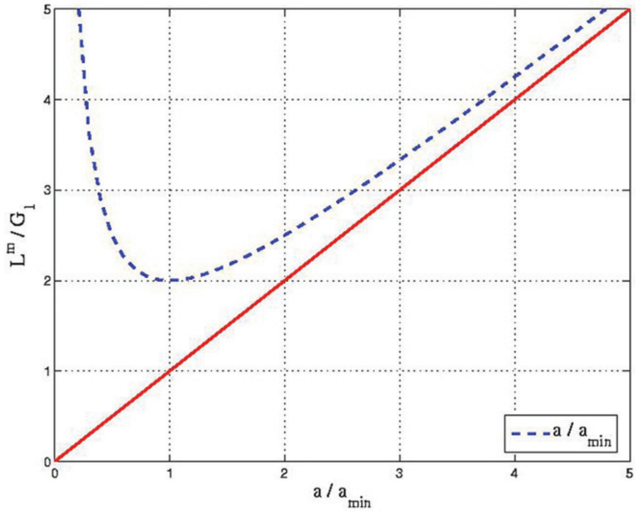

Figure 2. The normalized driving force $L^m/L^m_{\min}$ vs. $a/a_{\min}$.

even when there is not too much bond breaking, i.e. (a → 0), dislocations may still be present. The competition of these two factors dictates the overall behaviour of the driving force.

3. Multiscale Griffith criterion

A fundamental task of fracture mechanics is to determine the critical stress, $\tau_{\rm cr}$, under which the crack advances. Based on the Griffith criterion [2], the critical stress can be obtained by an equilibrium condition – the balance of configurational force and resistance force.

Following Griffith's energetic argument, we equate the multiscale driving force to the resistance,

$$L^m = \left(\frac{\pi a}{2\mu}\right)(\tau_{\rm cr})^2 + \left(\frac{3\ell^2\pi\tau_0^4}{8\mu a}\right)\frac{1}{(\tau_{\rm cr})^2} = 2\gamma_t. \tag{18}$$

We observe that the multiscale driving force has two parts: (1) the coarse-scale part, i.e. the release of elastic strain energy, or the value of the J-integral in the homogenized elastic medium, $\bar{J} = \pi a(\tau_{\rm cr})^2/2\mu$ and (2) the fine-scale part due to the release of the elastic free-energy stored inside the dislocation distribution zone, or the plastic zone, $L = (3\ell^2\pi\tau_0^4/8\mu a\tau_{\rm cr}^2)$. Note that in the multiscale Griffith equation the first part of the driving force may no longer be equal to the resistance due to surface separation, i.e. $2\gamma_s$. In other words, the strain energy release due to the reduction of the elastic potential in the elastic region will not be solely consumed in surface separation. To expedite the analysis, we introduce a

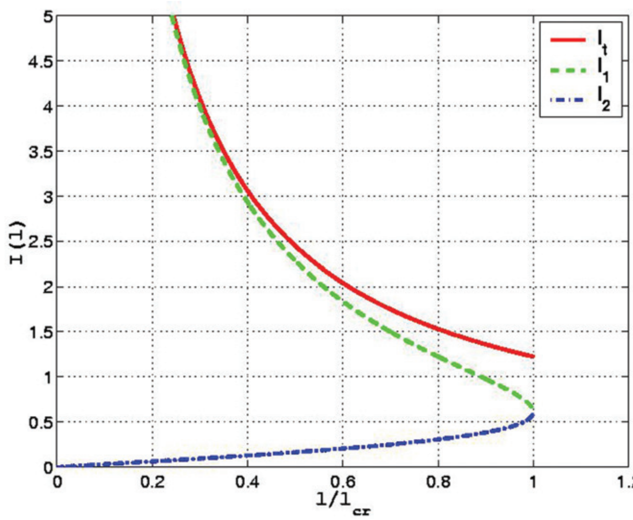

Figure 3. Bifurcated solutions for energy releases $I_i(\ell)$, $i = 1$, 2 and $I_t(\ell)$ vs. ℓ/ℓ_{cr}.

critical length-scale, $\ell_{cr} := 4/\sqrt{3}(\gamma_t\mu/\pi\tau_0^2)$, which is a function of the total resistance, elastic constant, and magnitude of the yield stress. Hence its value depends on the resistance curve commonly referred to as the R-curve, e.g. [17]. If we scale the energy release with a reference resistance energy, $2\gamma_0 := \pi\ell\tau_0^2/2\mu$, which may be viewed as the fracture resistance that the theoretical strength of the material can offer for ideally brittle fracture, the ratio

$$I(\ell) := \frac{\bar{J}}{2\gamma_0} = \left(\frac{a}{\ell}\right)\left(\frac{\tau_{cr}(a)}{\tau_0}\right)^2 \tag{19}$$

is a function of the length-scale ℓ. The symbol I is in honour of G.R. Irwin. Subsequently, the multiscale Griffith equation (18) is normalized as

$$I(\ell) + \frac{3}{4}\frac{1}{I(\ell)} = \frac{4\gamma_t\mu}{\pi\ell\tau_0^2} = \sqrt{3}\left(\frac{\ell_{cr}}{\ell}\right). \tag{20}$$

Unlike the classical Griffith equation, the multiscale Griffith equation is a quadratic equation in terms of energy release $I(\ell)$. Consequently, the multiscale Griffith equation (20) yields two solutions:

$$I(\ell)_{1,2} = \frac{I_t(\ell)}{2}\left[1 \pm \sqrt{1 - \left(\frac{\ell}{\ell_{cr}}\right)^2}\right] = \left(\frac{\gamma_t}{2\gamma_0}\right)\left[1 \pm \sqrt{1 - \left(\frac{\ell}{\ell_{cr}}\right)^2}\right] \tag{21}$$

where $I_t(\ell)$ is the normalized total resistance at the equilibrium,

$$I_t(\ell) = \gamma_t/\gamma_0 = \sqrt{3}\left(\frac{\ell_{cr}}{\ell}\right). \tag{22}$$

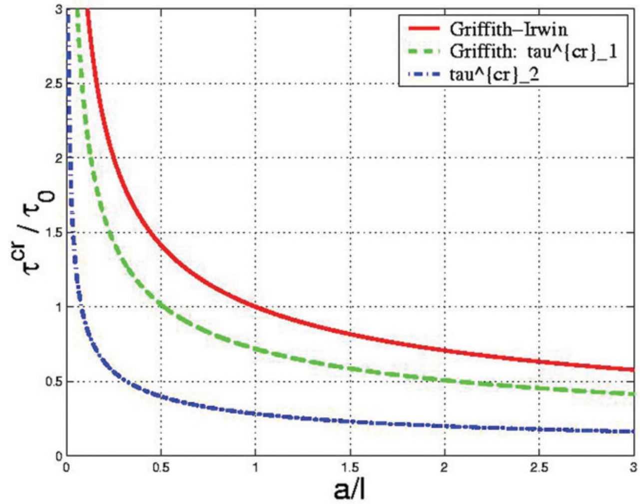

Figure 4. The critical stresses vs. a/ℓ at $\ell/\ell_{cr}=0.9$: (a) the Griffith–Irwin τ_I^{cr}/τ_0; (b) the first multiscale (Griffith) solution τ_1^{cr}/τ_0; and (c) the second multiscale solution τ_2/τ_0.

To compare the different energy releases, we plot the three normalized energy releases, $I_i(\ell)$, $i=1,2$ and $I_t=I_1+I_2$ in figure 3. One sees that the first two solutions of I_i bifurcate at $\ell=\ell_{cr}$. Using the definition (19), we find the corresponding critical stresses as follows,

$$\tau_{1,2}^{cr}=\tau_0\sqrt{\frac{\ell I_{1,2}(\ell)}{a}}=\sqrt{\frac{4\mu\gamma_t}{a\pi}}\left[\frac{1}{2}\left(1\pm\sqrt{1-\frac{\ell}{\ell_{cr}}}\right)\right]^{1/2}=\tau_I^{cr}f(\ell)_{1,2} \tag{23}$$

where $\tau_I^{cr}:=\sqrt{4\mu\gamma_t/a\pi}$ denotes the critical Irwin stress, and the scaling factors are defined as

$$f_{1,2}(\ell):=\left[\frac{1}{2}\left(1\pm\sqrt{1-\frac{\ell}{\ell_{cr}}}\right)\right]^{1/2}\leq 1.0 \tag{24}$$

which are functions of the length-scale parameter ℓ/ℓ_{cr}. In figure 4, the critical stresses corresponding to the multiscale Griffith criterion are compared with the Griffith–Irwin stress.

At equilibrium, the energy release solutions can be interpreted as either the driving forces or the resistances. To explore the physical meanings of the two solutions, we examine the asymptotic expressions of the critical stresses related to $I_{1,2}(\ell)$:

$$\tau_1^{cr}=\tau_I^{cr}f_1(\ell)\approx\sqrt{\frac{4\gamma_t\mu}{\pi a}}+\mathcal{O}(\ell),\quad\text{and}\quad\tau_2^{cr}=\tau_I^{cr}f_2(\ell)\approx\sqrt{\frac{3\pi\ell^2\tau_0^2}{16a\gamma_t\mu}}+\mathcal{O}(\ell^2). \tag{25}$$

One can find that the stress corresponding to $I_1(\ell)$ is independent of the yield stress, τ_0. This indicates that the first solution, $I_1(\ell)$, may be related to the resistance due to surface separation, i.e. $I_1(\ell)\sim\gamma_s/\gamma_0$, where γ_s is the resistance due to surface separation, whereas one may find in (25) that τ_2 depends on the yield stress τ_0, and hence we identify that $I_2(\ell)$ corresponds to the resistance due to incompatible defect fields, or the dislocation field. That is $I_2(\ell) \sim \gamma_{\rm p}/\gamma_0$, where γ_p denotes the energy dissipation due to the presence of dislocations. Fortuitously, the two roots of the multiscale Griffith equation (21) have an interesting property:

$$I_1(\ell) + I_2(\ell) = I_t(\ell) = \frac{\gamma_t}{\gamma_0}. \tag{26}$$

Since at equilibrium (in general, it is not true) both I_1 and I_2 can be viewed as resistance forces, therefore, Equation (26) suggests that the fracture resistance can also be expressed in a form of an additive decomposition (the sum of two resistances),

$$\gamma_t = \gamma_s + \gamma_p \Rightarrow \tau_I^{\rm cr} = \sqrt{\frac{4\mu(\gamma_s + \gamma_p)}{a\pi}} \tag{27}$$

which is the essential result of Irwin's multiscale theory of elastoplastic fracture under small-scale yielding. To the best knowledge of the author, this is the first rigorous proof or justification of Irwin's theory [18] by using multiscale analysis and continuum theory of dislocations.

Since $\tau_I^{\rm cr} \geq \tau_1^{\rm cr}$, $\tau_2^{\rm cr}$, it is natural to choose the Griffith–Irwin stress as the critical stress for its capture combined effects of $\tau_1^{\rm cr}$ and $\tau_2^{\rm cr}$ as exactly what G.R. Irwin did half a century ago. One may view $\tau_1^{\rm cr}$ as an approximation of the original Griffith stress for purely brittle fracture, and figure 4 shows how it compares with the Griffith–Irwin stress $\tau_I^{\rm cr}$.

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