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Understanding cracked materials: is Linear Elastic Fracture Mechanics obsolete?

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Abstract

Linear Elastic Fracture Mechanics has enabled the research community to solve a wide variety of problems of practical and scientific interest; however, it has historically suffered from two main shortcomings. Firstly, it predicts physically unrealistic singular stresses and strains at crack tips. Secondly, microstructural effects are lacking, so that a major source of size-dependent behaviour is not captured. Gradient-enriched elasticity overcomes both these shortcomings: singularities are avoided, so that crack-tip stresses can be used to assess integrity, and the inclusion of microstructural terms implies that size effects can be captured. In this investigation, it is shown that gradient-enriched crack tip stresses can directly be used to model the transition from the short to the long crack regime. The accuracy of this approach was validated by a wide range of experimental results taken from the literature and generated under both static and high-cycle fatigue loading. This high level of accuracy was achieved without having to resort to phenomenological model parameters: the extra constitutive coefficient was simply the (average) grain size of the material.

Keywords: Gradient elasticity, length scale, grain size

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Introduction

In 1964, Irwin affirmed that *"… linear elastic fracture mechanics already provides a rather complete set of mathematical tools. Additional experimental observations rather than additional methods of analysis are now the primary need for practical applications"* [1]. This has been taken quite literally: Linear Elastic Fracture Mechanics (LEFM) is still widely used, but its theoretical foundations have remained virtually untouched, being treated as axiomatic by the international scientific community. Therefore, most research efforts have been focussed on providing experimental data for a wide range of materials under different loading conditions. What we have achieved in sectors such as, for instance, transportation and energy production would have been impossible without the LEFM based design theories. There are, however, two main problems with LEFM: (i) singularities and (ii) microstructurally induced scale effects.

First of all, LEFM is based on the classical equations of elasticity, which predict singular stresses and strains at the tips of sharp cracks, re-entrant corners and other parts of the geometry that see an abrupt change of boundary conditions [2]. However, since at a macroscopic level *natura non facit saltus*, the appearance of singularities is an artefact. This is also supported by the fact that cracks in real materials experience the so-called blunting phenomenon – this holding true independently of the level of brittleness.

Secondly, LEFM does not capture the behaviour of short cracks [3], where "short" is to be understood in relation to the microstructural dimensions of the material (for instance the grain size of a metal)- see Refs [4, 5] and references reported therein. Indeed, the microstructural characteristics are missing from the elastic constitutive equations that form the basis of LEFM. This observation can be used (i) to understand why LEFM fails in describing short cracks, and (ii) which approach should be used instead. If the crack length is long compared to the microstructural dimensions, then the crack dominates the macroscopic behaviour and the microstructure can safely be disregarded without significant loss of accuracy. On the other hand, if the crack length is short compared to the microstructural dimensions, then crack and microstructure are equally important to predict the macroscopic behaviour.

Perhaps slightly crudely it can be said that LEFM has been developed to model the presence of zero-radius geometrical features according to classical linear elasticity, rather than tackling the roots of the problem, i.e. the material constitutive law. In this setting, a radically different approach would then be to revisit the basic ingredients of LEFM, that is the equations of classical elasticity, by including additional microstructural terms. With this microstructural enrichment, the equations of elasticity can be used effectively to describe the short- as well as the long-crack behaviour. This obviously implies that this idea can only be used provided that the plasticity effects can be neglected with little loss of accuracy (such as, for instance, in brittle materials and in metals cracking in the high-cycle fatigue regime).

Fundamentals of gradient-enriched elasticity

Gradient elasticity is understood here as a subclass of so-called “generalised continuum” models in which microstructural terms are included in the classical equations of elasticity. More particularly, in gradient elasticity higher-order spatial derivatives of relevant state variables (such as strains, stresses or accelerations) appear. In what follows, we will assume quasi-static conditions; that is, inertia contributions are left out of consideration.

The first systematic treatise of gradient elasticity is due to Mindlin [6]. He started off by deriving a mathematically complete but rather complicated theory of elasticity with microstructure and 903 independent constitutive coefficients, which he then simplified to an isotropic gradient elasticity theory with 2 standard coefficients (the usual Lamé constants) and two length parameters that account for the microstructural effects. A few decades later, an even simpler theory was suggested by Aifantis, whereby the relation between stresses, σ, and strains, ε, is written as [7-13]

$$\sigma = C : \left(\varepsilon - \ell^2 \nabla^2 \varepsilon \right) \tag{1}$$

where C is a fourth-order tensor containing the usual elastic moduli. The only new parameter compared to classical elasticity is the length scale parameter ℓ, and it is clear that the standard equations of elasticity are retrieved by taking $\ell = 0$.

The actual solution of a boundary value problem with the enriched constitutive relation of Eq. (1) is most conveniently performed using the solution method devised by Ru and Aifantis [12] and later extended to finite element implementations [14]. In this Ru-Aifantis approach, firstly the classical equations of elasticity are solved by ignoring the effects of the length parameter. Afterwards, the stresses (or strains, or displacements – see [14] for a discussion) are used in a pseudo reaction-diffusion equation that includes the length parameter and that leads to a smoothing of the relevant fields. Thus, the singular stresses that are found using classical elasticity at the tips of sharp cracks are transformed into finite (yet localised) stresses after this second step of the analysis is performed. It is emphasized that both steps of the analysis (i.e. the standard elastic analysis followed by the stress-smoothing) involves the solution of a global system of linear equations. Thus, the computational costs are roughly double that of performing a standard elastic analysis.

The length parameter ℓ has in the literature (see for instance [8] for an overview) been linked to a wide variety of microstructural quantities ranging from the inter-particle spacing in an atomic lattice to the laminate thickness in composites. Obviously, there are several orders of magnitude difference in such estimates, but a general conclusion from the overview in [8] is that the length parameter ℓ is related to the size of the *dominant* source of heterogeneity. This can probably best be captured by linking ℓ to the Representative Volume size L_{RVE} for a heterogeneous material, i.e. [15]

$$\ell^2 = \frac{1}{12} L_{RVE}^2 \qquad (2)$$

In an elastic context, the Representative Volume size is normally found to be equal to a few times the average size of the dominant inclusion [9, 10]. For the ceramic and metal materials used in the experimental validation below, this would be the *grain size.* Thus, for such materials it follows that the intrinsic length scale parameter ℓ of gradient elasticity is roughly of the same magnitude as the grain size of the material.

Embedding strength in gradient elastic stress analysis: a novel method to assess cracked materials

The fact that stresses and strains are non-singular in gradient elasticity has an important implication for fracture mechanics: namely, the stresses at the crack tip can be used directly to assess the integrity of the material or the structural component. Therefore, *strength analysis* follows straightforwardly from *stress analysis,* which is in contrast with LEFM. The mathematical intricacies of LEFM (such as the *J*-integral and stress intensity factors) can thus be avoided altogether, whilst the linear structure of the equations (and the associated simplicity of analytical and numerical solution procedures) is maintained. Consequently, the integrity of materials and structural components can be assessed in a much more intuitive, robust and generalised way.

A new result in this context is the unified treatment of static and fatigue-induced cracks for a large range of crack lengths. Consider the plate containing a central through-thickness crack which is sketched in Figure 1. If such a plate is subjected to a static axial force, the resulting nominal gross stress is equal to σ_g. In a similar way, when the above cracked plate is subjected to a cyclic force, the range of the corresponding nominal gross stress is denoted as $\Delta\sigma_g = \sigma_{g,\max} - \sigma_{g,\min}$, where $\sigma_{g,\max}$ and $\sigma_{g,\min}$ are the maximum and minimum nominal gross stress in the fatigue cycle, respectively.

With gradient elasticity, the corresponding stress field can then be determined by directly incorporating into the stress analysis the length scale parameter ℓ. This allows the gradient-enriched crack tip stress to be determined under both static (σ_{tip}) and fatigue loading ($\Delta\sigma_{tip}$) – see Figure 1. By using the Theory of Critical Distances argument [4, 16], the assumption can be formed that crack propagation is inhibited as long as the following conditions are assured:

$$\sigma_{tip} \leq \sigma_{UTS} \qquad \text{(static assessment)} \qquad (3)$$

$$\Delta\sigma_{tip} \leq \Delta\sigma_0 \qquad \text{(high-cycle fatigue assessment)} \qquad (4)$$

where σ_{UTS} is the material ultimate tensile strength, whereas $\Delta\sigma_0$ is the un-notched material fatigue limit experimentally determined under the same load ratio $R=\sigma_{g,\min}/\sigma_{g,\max}$ as the one characterising the in-service load history applied to the cracked material being assessed.

Another important aspect which is worth mentioning here is that the intrinsic length scale parameter ℓ of gradient elasticity is directly related to the classic LEFM material properties [16, 17] through the following critical distances [4]:

$$L_S = \frac{1}{\pi}\left(\frac{K_{Ic}}{\sigma_{UTS}}\right)^2 \qquad \text{under static loading} \qquad (5)$$

$$L = \frac{1}{\pi}\left(\frac{\Delta K_{th}}{\Delta\sigma_0}\right)^2 \qquad \text{under high-cycle fatigue loading} \qquad (6)$$

In the above definitions, K_{Ic} is the plane strain fracture toughness, whereas ΔK_{th} is the threshold value of the LEFM stress intensity factor range. By using the Area Method argument re-interpreted according to non-local mechanics, it was then shown that intrinsic length scale parameter ℓ can directly be estimated via the above critical distance values as follows [16, 17]:

$$\ell \approx \frac{1}{8}L_S \qquad \text{under static loading} \qquad (7)$$

$$\ell \approx \frac{1}{8}L \qquad \text{under high-cycle fatigue loading} \qquad (8)$$

Relationships (7) and (8) should make it evident that there exists an implicit link between gradient elasticity's and LEFM's *modus operandi,* even though gradient elasticity allows the static and high-cycle fatigue assessment to be performed without making use of K_{Ic} and ΔK_{th}, respectively. This will be proven in the next section.

To conclude, it also worth observing that, in the log-crack regime, gradient elasticity is seen to be able to model the scale effect in accordance with what postulated by LEFM. In particular, in Refs [16, 17] it was proven that, when ℓ is estimated via Eqs (7) and (8), the use of gradient-enriched crack tip stresses results, in a Kitagawa-Takashi like log-log representation, in a straight-line having inverse slope equal to -1/2 and perfectly overlapping the threshold straight line estimated according to LEFM.

Experimental validation

By performing a systematic bibliographical investigation, a number of relevant experimental results were selected from the technical literature. All data re-analysed in the present section were generated by testing samples under both static and cyclic loading. The specimens tested under *static loading* were made of different ceramic materials with crystalline structure. In such materials, atoms are linked together mainly either by ionic bonds (such as Al_2O_3) or by covalent bonds (such as SiO_2). Since both ionic and covalent bonds are characterised by a high lattice resistance to the dislocation motion, fast fracture in cracked ceramics is seen to occur mainly trans-granularly due to cleavage [18]. Table 1 summarises the static mechanical properties of the investigated ceramics with the corresponding average grain size d , where K_{Ic} is the plane strain fracture toughness (as to the experimental determination of both d and K_{Ic}, the Reader is referred to the original sources). The experimental data were obtained under axial loading by testing samples containing different crack-like geometrical features, including controlled surface flaws, surface scratches, large pores, and sharp notches. Such results were generated by employing either cylindrical or flat specimens having reference dimensions of the cross sectional area in the range 3-10 mm.

The cracked specimens tested under *high-cycle fatigue loading* were instead made of two different metallic materials, i.e. 2.25Cr-1Mo [27] and JIS SM41 [28, 29]. Table 2 lists the fatigue properties of the above metals together with the corresponding average grain size d (as reported in the quoted papers). Further, in this table also the threshold values of the LEFM stress intensity factor range, denoted as ΔK_{th}, are reported, such material properties being experimentally determined under the appropriate value for load ratio R (as to the experimental procedures followed to determine ΔK_{th} the Reader is referred to the original sources). Finally, the re-analysed experimental results were generated by testing, under cyclic axial loading, cylindrical samples of 2.25Cr-1Mo [27] containing superficial cracks and plates of JIS SM41 containing lateral cracks [28, 29]. The gauge length diameter of the 2.25Cr-1Mo specimens was equal to 10 mm [27], whereas the 2.25Cr-1Mo rectangular specimens with two lateral cracks had gross cross-sectional area equal to 50 x 3 mm [28, 29].

From a cracking behaviour point of view, similar to what is observed in ceramics loaded statically, also in metals at room temperature fatigue cracks are seen to grow mainly in a trans-crystalline mode [30]. Further, in terms of crack arrest mechanisms, both in ceramics loaded statically and in metals subjected to fatigue loading, the propagation of cracks is seen to be arrested by the grain boundaries that act as inherent microstructural barriers [31, 32]. This supports the hypothesis, mentioned earlier, that the gradient elasticity length scale parameter ℓ is proportional (and in fact, as we argued, more or less equal) to the grain size d. Thus, we will use $\ell = d$.

The selected experimental results are summarised in the normalised Kitagawa-Takashi diagram [3] reported in Figure 2. For static failure, the vertical axis is the ratio between the nominal gross stress resulting in the breakage of the ceramic samples, σ_{th}, and the material ultimate tensile strength, σ_{UTS}. For fatigue failure, the ordinate is the ratio between the range of the nominal fatigue limit (referred to the specimens' gross section), $\Delta\sigma_{th}$, and the material un-notched fatigue limit, $\Delta\sigma_0$. This parametrisation allows results generated under static and high-cycle fatigue loading to be plotted in the same chart. The horizontal axis is the normalised equivalent crack length calculated as $F^2 a / d$, where F is the LEFM geometric shape factor of the specimen and a is the crack length. The equivalent length defined as above allows experimental results generated by testing samples having shape factor F different from unity to be compared directly to the case of a central crack in an infinite plate loaded in tension (for which F is, by definition, equal to unity) [33]. In other words, in Figure 2 the LEFM shape factor F is used solely to summarise in a single diagram data from samples with different geometries; F is not related to the material parameters.

These experimental data are accompanied by the results of numerical modelling; the curve plotted in Figure 2 was determined numerically by sampling the gradient enriched stresses at the tip of the crack – something that would be impossible in LEFM, as these stresses would then be singular. The numerical results were obtained through two consecutive steps of numerical analysis. First, a standard linear elastic analysis was performed, leading to a displacement field in which all gradient effects are absent. Next, the displacements found in the first step are used as input in the second step, in which a reaction-diffusion type equation is solved on the same finite element mesh to introduce the gradient enrichment and, thus, the effects of the micro-structural length. Similar to the first step, in the second step a global system of equations must be solved, but the unknowns in the second step are the gradient-enriched stresses (for full details, see [8, 10]).

Turning back to the chart of Figure 2, the threshold condition (continuous curve) was determined by recalculating the nominal stress (i.e. either σ_{th} or $\Delta\sigma_{th}$) so that $\sigma_{tip} = \sigma_{UTS}$ for static loading and $\Delta\sigma_{tip} = \Delta\sigma_0$ for fatigue loading, respectively – see Eqns (3) and (4). The diagram of Figure 2 makes it evident that gradient enriched crack tip stresses are successful in modelling the transition from the short- to the long-crack regime, this holding true both under static and fatigue loading.

Discussion

It is well-known that LEFM cannot be used to model the behaviour of short cracks. For any material, LEFM predicts that the nominal strength increases as the crack length decreases, eventually resulting in a failure stress which is higher than either the material ultimate tensile strength σ_{UTS} (under static loading) or the plain fatigue limit $\Delta\sigma_0$ (under high-cycle fatigue loading). In contrast, as can be verified from Figure 2, gradient-enriched elastic crack tip stresses are capable of capturing the transition from the short to the long-crack regime. For decreasing crack lengths, the gradient-enriched crack tip stresses gradually approach the horizontal asymptote given by the inherent material strength. Note also that the right-hand side straight branch of the curve plotted in the normalised Kitagawa-Takashi diagram is characterised by a slope equal to $-1/2$, which is in accordance with the LEFM basic equations, i.e. $K = F \cdot \sigma_g \sqrt{\pi a}$ for static failure or $\Delta K = F \cdot \Delta\sigma_g \sqrt{\pi a}$ for fatigue failure.

From a practical point of view, the real novelty here is that accurate predictions can be made by simply using the grain size d and either the material ultimate tensile strength σ_{UTS} or the plain fatigue limit $\Delta\sigma_0$, without any additional curve fitting. This results in great simplification of the design process, since experimentally determining both K_{Ic} and ΔK_{th} according to the pertinent standard codes' procedures is not only expensive, but also time-consuming. In contrast, with gradient elasticity, structural integrity can be assessed without the need for determining K_{Ic} or ΔK_{th} at all.

It is also worth observing that the majority of the experimental results fall within an error interval of ±20%. Such a physiological scattering can be ascribed, on one hand, to the well-known difficulties which are usually encountered when manufacturing and testing cracked specimens (especially those containing short cracks), and, on the other hand, to the actual material morphology as well as on the presence of both microstructural defects and hard inclusions [4]. The level of conservatism which is obtained in the very long-crack regime deserves to be discussed in detail. In the presence of very long cracks, the effect of the cracks themselves tends to prevail over the local effect of the microstructure. Accordingly, the level of conservatism which is obtained in the very long-crack regime could be ascribed to the fact that when cracks become very long compared to the material microstructural features, the size of the process zone may change, resulting in a different value for length scale ℓ: the validity of this idea is supported by the fact that slightly reducing the value of critical length ℓ (i.e. taking $\ell = 0.75 \cdot \mathrm{d}$) would have been enough to accurately predict the experimental results also in the very-long crack regime. However, using the grain size d allows the long-crack behaviour to be modelled by reaching a slightly higher margin of safety.

Using gradient elastic facture mechanics instead of LEFM can have significant impact on materials science. Similar to what is commonly done with finite radius stress raisers, design stresses are directly estimated at the crack tips, that is, at those material points for which LEFM would predict infinitely large stresses. Both static and high-cycle fatigue strength can be estimated by solely using those mechanical properties which are usually available for engineering materials, i.e. the material ultimate tensile strength and the plain fatigue limit. The fact that the necessary stress fields are directly determined through conventional finite element models implies that practitioners with no specific LEFM background can safely and efficiently design cracked material against either static or high-cycle fatigue loading.

Conclusions

- Using gradient elasticity instead of classical elasticity, stress analysis is still elastic, but singularities due to abrupt changes in boundary conditions can be avoided.
- Singular-free stress fields imply that crack tip stresses are unique and finite, and can thus be used for design directly. Hence, strength analysis can be merged into stress analysis.
- Through the inclusion of an internal length parameter, the effects of microstructure enter the stress analysis. This accounts for size and scale effects, and thus a unified description of long and short cracks is possible.

- We have validated our methodology with a number of experimental results. These have confirmed its capability to model the transition from the short to the long crack regime under static as well high-cycle fatigue loading. However, more work is obviously required to check the applicability of our approach to other fracture-related problems.
- In anticipation of future work, being able to use crack tip stresses has the potential to change radically the way the behaviour of cracked materials is modelled.

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List of Captions

Table 1: Mechanical static properties, and grain size d, of the investigated engineering ceramics.

Table 2: Fatigue properties, and grain size d, of the investigated metallic materials.

Figure 1: In-field use of gradient-enriched crack tip stresses to perform both the static and the high-cycle fatigue assessment of cracked materials.

Figure 2: Accuracy of gradient-enriched crack-tip stresses in modelling the transition from the short to the long-crack regime under both static and fatigue loading.

Tables

Material	Ref.	σ_{UTS} [MPa]	K_{Ic} [MPa·m$^{1/2}$]	d [mm]
SiC	[19]	620	3.7	0.003
Sialon	[19]	920	4.6	0.002
Si_3N_4	[19]	650	4.5	0.004
Si_3N_4	[20, 21]	880	5.0	0.0015
Si_3N_4	[22]	700	5.0	0.0015
Si_3N_4	[23]	700	5.0	0.0030
Si_3N_4	[24]	510	5.0	0.004
Al_2O_3	[19]	200	3.1	0.02
Al_2O_3	[20]	790	3.5	0.003
Al_2O_3	[20]	610	3.5	0.007
Al_2O_3	[23]	210	3.5	0.02
Al_2O_3	[25]	610	3.5	0.002
Al_2O_3	[25]	390	3.5	0.005
Al_2O_3	[26]	390	3.5	0.003

Table 1: Mechanical static properties, and grain size d, of the investigated engineering ceramics.

Material	Ref.	R	$\Delta\sigma_0$ [MPa]	ΔK_{th} [MPa·m$^{1/2}$]	d [mm]
2.25Cr-1Mo	[27]	-1	502	12.6	0.1[a]
JIS SM41	[28, 29]	-1	331	13.0	0.025
JIS SM41	[28]	0	310	6.5	0.025
JIS SM41	[28]	0.5	271	4.6	0.025

[a]Austenite grain size

Table 2: Fatigue properties, and grain size d, of the investigated metallic materials.

List of Captions

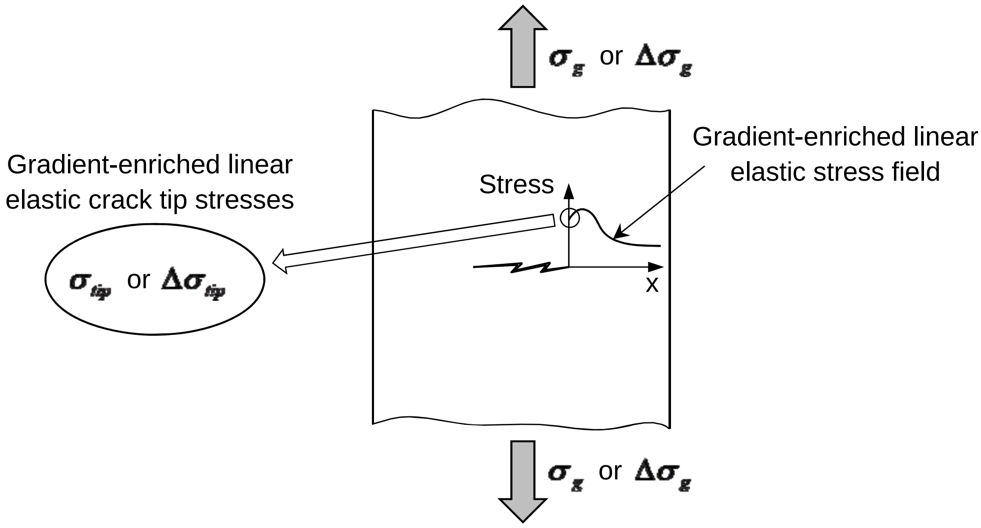

Figure 1: In-field use of gradient-enriched crack tip stresses to perform both the static and the high-cycle fatigue assessment of cracked materials.

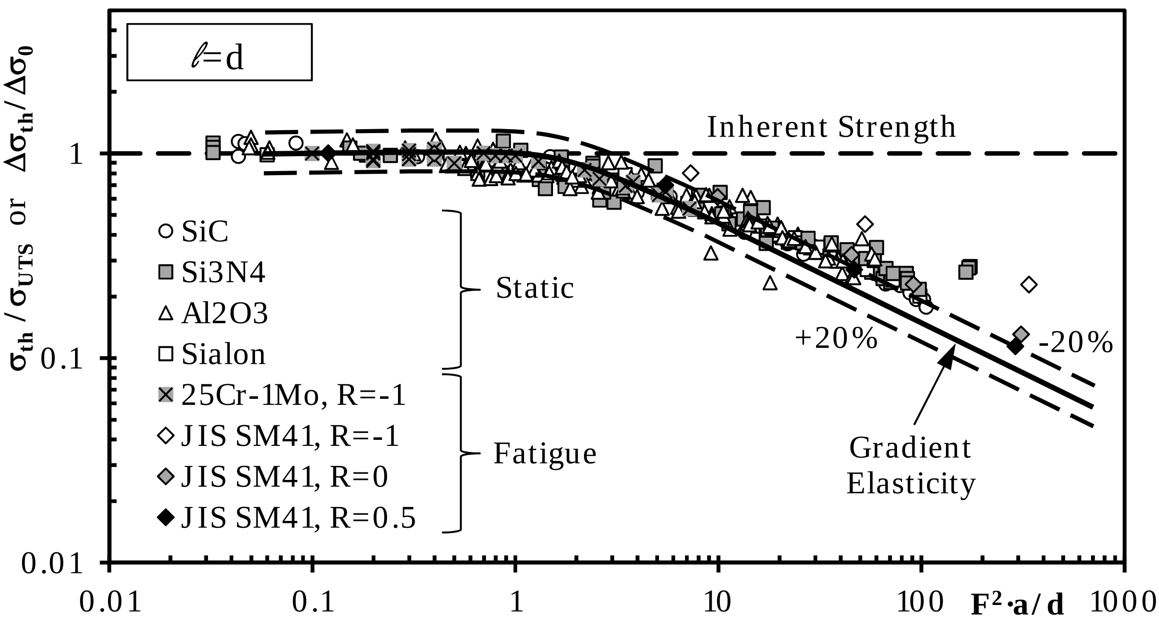

Figure 2: Accuracy of gradient-enriched crack-tip stresses in modelling the transition from the short to the long-crack regime under both static and fatigue loading.