Modelling the Plane Strain Fracture Toughness of Titanium and Aluminium alloys at Room Temperature

The processes of material manufacturing, processing, machining, and forming may introduce flaws in a finished mechanical component. Flaws can appear as cracks, voids, metallurgical inclusions, weld defects, design discontinuities, or some combinations of them. Fracture toughness is a property which describes the ability of a material to resist fracture. This report provides a brief overview of fracture toughness and the model used in JMatPro® v11 to calculate this property for titanium and aluminium alloys at room temperature.

Stress Intensity Factor (SIF) and Failure Criteria

In fracture mechanics, there are three ways of applying a force to enable a crack to propagate (Fig. 1): opening (mode I), sliding (mode II) and tearing (mode III), with mode I receiving the majority of research interest. The stress state near the tip of a crack caused by a remote load can be predicted by a parameter called the stress intensity factor K. The magnitude of K depends on sample geometry, the size and location of the crack, and the magnitude of loads on the material. It can be represented by the following typical expression

$$K = Y\sigma\sqrt{\pi a} \tag{1}$$

where *a* is the crack length, σ is the remotely applied stress and *Y* is a dimensionless component geometry factor. Unstable fast fracture occurs when *K* approaches a critical value named the fracture toughness *K*_C, with the unit $MPa\sqrt{m}$ or $ksi\sqrt{in}$. Knowledge of fracture toughness can be of practical assistance in two aspects:

- (1) To determine the critical crack length when a given stress is applied to a component;
- (2) To determine the critical stress value when a given crack length is found in a component.



Figure 1 Typical modes of fracture ^[1]

Plane Strain Fracture Toughness

Fracture toughness K_C varies with thickness (*B*) of specimens, because the stress concentration adjacent to the flaw increases with thickness, from plane stress to plane strain condition. When the thickness exceeds some critical dimension, K_C is found to be relatively constant (independent of the crack geometry and loading), which is then a true fundamental material property called plane strain fracture toughness K_{IC} (Fig. 2). An accurate determination of the plane strain fracture toughness requires a specimen to have a thickness *B*

$$B \ge 2.5 \left(\frac{K_{IC}}{\sigma_y}\right)^2 \tag{2}$$

where σ_y is the yield strength. Note that the plane strain condition is a rather idealized condition thus the value of K_{IC} may be conservative in reality. However, in practice, this conservative value can provide more safety and confidence to engineers in their design applications. In the following context we simply use "**fracture toughness**" to represent the property "**plane strain fracture toughness**".



Figure 2 Role of material thickness to fracture toughness^[1]

Modelling of Fracture Toughness

In linear elastic and elasto-plastic fracture mechanics (LEFM and EPFM), the fracture toughness K_{IC} has been correlated to many other equivalent properties, such as energy release rate (in LEFM and EPFM), *J*-integral and crack tip opening displacement (CTOD, in EPFM). Determination of K_{IC} from the energy release rate or *J*-integral requires either experimental measurements or numerical simulations. The critical CTOD (δ_c) has a well-established relationship with the fracture toughness at plane strain condition:

$$\delta_C = \frac{\sigma_y}{2E'} \left(\frac{K_{IC}}{\sigma_y}\right)^2 = \frac{K_{IC}^2}{2E'\sigma_y} \tag{3}$$

where *E*' is a correction of the elastic modulus for plane strain condition, $E' = E / (1-v^2)$, and *v* is Poisson's ratio. Based on this, together with investigations of extensive metallurgical evidence ahead of a crack tip in different materials, Hahn and Rosenfield ^[2] proposed a critical strain based fracture criteria and derived an analytical model (here we call it HR model) that correlates K_{IC} with ordinary tensile properties of ductile metals at room temperature:

$$K_{IC} \approx \sqrt{2E'\sigma_y n^2 \varepsilon_f} \quad (ksi\sqrt{in}) \quad \text{or} \quad K_{IC} \approx \sqrt{0.05 \cdot E'\sigma_y n^2 \varepsilon_f} \quad (MPa\sqrt{m}) \quad (4)$$

where *n* is the strain hardening exponent and ε_f is a critical fracture strain localized to the crack tip, as geometrically and mechanistically correlated to δ_c . Note that the HR model is consistent with another model proposed by Robert Ritchie reported more recently ^[3], where n^2 can be treated as a characteristic width of the plastic zone ahead of the crack tip. The model does not contradict the common trend for a given material such that K_{IC} decreases with increasing σ_y . Generally, the value of *n* is seen to decrease with increasing σ_y , and microstructural changes which enhance σ_y would also cause a more rapid reduction in ε_f . Therefore, the influence of an increasing σ_y on K_{IC} can be counteracted by a decreasing *n* and ε_f .

In the original work by Hahn and Rosenfield ^[2], a further empirical correlation is made between the critical fracture strain ε_f and the elongation obtained from a standard tensile test, considering that the ductility is expected to reduce from the unnotched plane strain condition to that ahead of a crack due to the high stress triaxiality. The model has been shown to predict reasonable K_{IC} values compared with experiment (within 30% limit) across different aluminium, steel and titanium alloys ^[2]. However, the correlation with elongation seems to be disputable because of the limited number of tests and the intrinsic uncertainty in the elongation measurements and predictions. Therefore, the critical fracture strain needs to be carefully assessed for many materials in each type of alloys before the model can be widely adopted. In this report, new phenomenological correlations of ε_f are explored for titanium and aluminium alloys, particularly with the respect to the different microstructural features.

Fracture Toughness of Titanium Alloys

The microstructure of titanium alloys is relatively simple, consisting of only Alpha and Beta matrix phases but few precipitates. Complexity, however, exists in the morphology of Alpha phase where acicular Alpha structure tends to be more resistant to fracture than equiaxed Alpha structure (Fig. 3), which is controlled by the type of heat treatment applied to the alloy.



Figure 3 Schematic diagram showing effect of alloy strength and microconstituents on toughness in titanium alloys^[4]

An extensive range of room temperature K_{IC} data of Acicular Alpha, Equiaxed Alpha, Beta, Acicular Alpha-Beta and Equiaxed Alpha-Beta titanium alloys subject to various heat treatment temperatures (300-1100°C) has been collected which justifies the trend with morphology and yield strength shown in Fig. 3. Here three groups of single phase alloys (Acicular and Equiaxed Alpha, Beta) are chosen for the correlation. The experimental K_{IC} and σ_y are used along with E, v and n calculated by JMatPro®, which are then substituted in Eq. (4) to back calculate ε_f . A correlation function is then extracted between ε_f and σ_y of each single phase alloy. The physics behind this is that, with the absence of precipitates, the void nucleation and crack propagation are mainly controlled by the localised stress state. In general, a high yield strength would lead to a low fracture strain.

For dual phase (Acicular Alpha-Beta and Equiaxed Alpha-Beta) titanium alloys, a critical fracture strain for each phase is firstly obtained from the corresponding correlation function with the respective yield strength. Then the actual critical fracture strain of the dual phase alloy is calculated using the following mixture law and the fraction of each phase calculated in JMatPro®

$$\varepsilon_f = f_{Alpha} \varepsilon_f^{Alpha} + \left(1 - f_{Alpha}\right) \varepsilon_f^{Beta} \tag{5}$$

Such a mixture law dictates a ductile strain-based micro-void coalescence behaviour in the different phases. Finally this fracture strain is substituted in Eq. (4) to calculate K_{IC} of each dual phase alloy. Figure 4(a) demonstrates the validity of the current approach at room temperature, comparing the calculated K_{IC} of all the collected alloys with experimentally measured values ^[5-9, 12-14]. The types of alloys are distinguished by different colours and shapes of the data points. The majority of the calculated results fall within 30% limit region from the measured value. Figure 4(b) provides an additional validation of the yield strength normalised K_{IC} . A reasonable agreement can be seen as all the points are close to the line of perfect match.



Figure 4 Comparison of calculated (a) standard, and (b) yield strength normalised fracture toughness of **Titanium alloys** with experimental measurements at room temperature.

Fracture Toughness of Aluminium Alloys

The microstructure of aluminium alloys is more complicated than titanium, consisting of the aluminium matrix phase, which contain a wide range of precipitate species. Variation in the processing methods (casting and wrought) also adds to the complexity in the subsequent mechanical behaviour. Compared with titanium alloys, a collection of fracture toughness data of casting and wrought aluminium alloys across different series does not exhibit a clear trend with yield strength (Fig. 5).



Figure 5 Experimental yield strength vs fracture toughness data of casting and wrought aluminium alloys across different series at room temperature.

A considerable literature on aluminium alloys have linked the voids nucleation, growth and coalescence for ductile fracture with the existence of coarse precipitates ^[26, 35-37], which largely appear after solution treatment or solidification. However, not all coarse particles have been found to be detrimental. In fact, the role of different precipitate phases in aluminium alloys has been investigated and classified ^[26, 35-37]. Apart from the large size, the detrimental particles must have low cohesiveness and large misfit with the matrix, which trigger stress concentration and defect accumulation around them. These particles are often called void-nucleating or void-initiating particles ^[26,35,37], or undesirable second-phase particles that serve as crack nucleation sites. Accordingly, the fracture strain/ductility has been understood to be a function of the volume fraction of the void-nucleating coarse precipitates ^[26,35,37]. While a dispute seems to exist in literature regarding the detrimental solute elements in these void-nucleating precipitates, a consensus is found in all works on two elements, Fe and Si, and such typical precipitates include Mg₂Si and Al₇Cu₂Fe.

Here the critical fracture strain ε_f in the Eq. (4) for aluminium alloys is firstly back calculated from the measured K_{IC} and σ_y data (Fig. 5), using the same procedure as for titanium alloys. Then ε_f is correlated with the volume fraction of void-nucleating coarse precipitates f_v containing Fe and Si, which is calculated by JMatPro®, either at the given solution treatment temperature or at the solidus given the solidification condition in literature (345-580°C). Note that casting and wrought alloys are correlated separately.

$$\varepsilon_f \propto f_v$$
 (6)

The correlation functions are then used to predict K_{IC} using the HR model (Eq. 4) and compare with the measured values. Figure 6 demonstrates the validity of the approach for the fracture toughness of aluminium alloys at room temperature (Fig. 6a compares K_{IC} and Fig. 6b compares K_{IC}/σ_y). The hollow points are for casting alloys while the solid points are for wrought alloys. Different series of alloys are distinguished by the colours and shapes of the data points. Similar agreement of the predictions with experiments as that of the titanium alloys in Fig. 4 can be seen.

Finally, it should be noted that for most types of titanium and aluminium alloys (Fig. 4a and Fig. 6a), apart from the \pm 30% limit, the variation of fracture toughness generally follows the slope of the line of the perfect match, giving reasonable agreement of the general trend. In addition, the enriched data collection of each type of alloy justifies the correlation function for the critical fracture strain, which enables to provide a more robust correlation with different microstructural features than the original work with the elongation.



Figure 6 Comparison of calculated (a) standard, and (b) yield strength normalised fracture toughness of **Aluminium alloys** with experimental measurements at room temperature.

Summary

The model used in JMatPro® v11 to calculate the plane strain fracture toughness K_{IC} of titanium and aluminium alloys at room temperature has been described. It links K_{IC} with ordinary tensile properties and, most importantly, different microstructural features, with Alpha-Beta phase fraction and morphology for titanium alloys, and void-nucleating undesirable coarse precipitates for aluminium alloys.

The approach requires only a limited number of user inputs, such as yield strength and heat treatment temperature. Reasonable agreement with the experimental results has been achieved for both titanium and aluminium alloys at room temperature. Considering the intrinsic scatter in the measurements of fracture toughness, which can be attributed to a number of aspects such as materials' anisotropy and localised heterogeneous microstructure distribution ahead of a crack tip, the current analytical approach could help reduce uncertainty and facilitate the assessment of the level of fracture toughness, and mitigate the lack of material data required for fracture process simulations.

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