# Microstructure based evaluation of material fracture toughness

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*Summary* A cohesive finite element method (CFEM) based multi-scale framework for analyzing the effects of microstructural heterogeneity, phase morphology, constituent behavior and interfacial bonding strength on the fracture toughness of materials is developed. The computational framework allows the fracture toughness to be predicted as functions of microstructural attributes and constituent behavior. The method uses the *J*-integral and the linear elastic relation between *J* and *K*.

## INTRODUCTION

The evaluation of material fracture toughness as functions of microstructure attributes is a fundamental issue in material science. It requires proper characterization of microstructures and quantitative correlation of microstructural attributes with overall material response. Experimental approaches allow systematic studies of microstructure-fracture toughness relations but fail to explore material configurations not yet in existence. Besides, the trial-and-error process is usually associated with high cost and long cycles. To overcome the above shortcomings, a cohesive finite element method (CFEM) based multi-scale framework for analysing the effect of microstructural heterogeneity, phase morphology, constituent behavior and interfacial bonding strength on the fracture toughness is developed as shown in Fig. 1. This framework allows explicit representation of microstructures and allows explicit representation of microstructures and account of microstructural level of deformation, damage and failure mechanisms, while allowing macroscopic conditions such as controlled loading and structural response to be considered at the same time. This framework provides a means for calibrating model parameters at the microscale through macroscale responses which can be easily measured in experiments. More importantly, it allows macroscopic response measures such as $K_{IC}$ to be evaluated as functions of microstructure by calculating the *J*-integral along an arbitrary contour within the homogenized region.

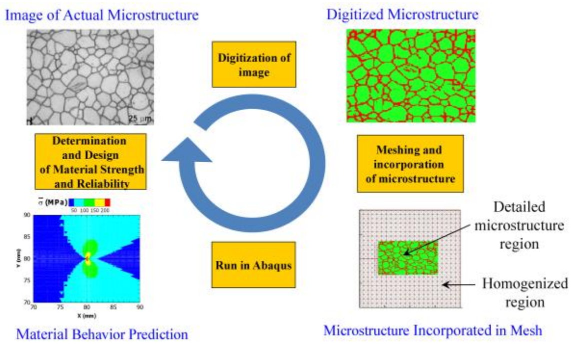


Fig. 1 The multi-scale CFEM framework for material design.

## *J*-INTEGRAL BASED FRACTURE TOUGHNESS EVALUATION

For the model shown in Fig. 1, contours for *J* evaluation are solely within the homogenized part of the specimen where no cohesive elements are used. For brittle materials, the *J*-integral is equivalent to the energy release rate *G* and can be related to the stress intensity factor *K* [1]. The generalized path-independent *J*-integral for dynamic conditions is used in this analysis as [2–4]

$$J = \int_{\Gamma} \left[ \left( \int_0^t \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon} + \frac{1}{2}\rho \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} \right) \mathrm{d}x_2 - \boldsymbol{t} \cdot \frac{\partial \mathbf{u}}{\partial x_1} \mathrm{d}s \right] + \int_A \left( \rho \ddot{\mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial x_1} - \rho \dot{\mathbf{u}} \cdot \frac{\partial \dot{\mathbf{u}}}{\partial x_1} \right) \mathrm{d}A, \tag{1}$$

where $\boldsymbol{t}$ is the traction on a surface with normal $\mathbf{N}$ in the reference configuration, $\mathbf{u}$ is the displacement, $\boldsymbol{\varepsilon}$ denotes the engineering strain and $\rho$ is the mass density.

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Fig. 2 shows six snap shots of the crack propagation process in a microstructure with circular $TiB_2$ reinforcement at a loading velocity of $v = 5$ mm/s. The corresponding histories of *J* and *K* are shown in the center. Fracture initiates in the $Al_2O_3$ matrix at 105.0 μs [Fig. 2(a)], this event defines the initiation toughness $K^i_{IC}$. The crack is arrested by a $TiB_2$ particle and pauses at the $Al_2O_3/TiB_2$ interface for approximately 42.5 μs [Fig. 2(b)]. During the pause, *J* increases rapidly. At approximately 149.2 μs [Fig. 2(c)], as a result of the higher level of driving force *J*, the crack penetrates the $TiB_2$ particle. Subsequently, the crack propagates rapidly, causing *J* (and therefore *K*) to plateau for the remainder of the analysis. The average value of *K* during this period is taken as the propagation toughness $K_{IC}$ [5].

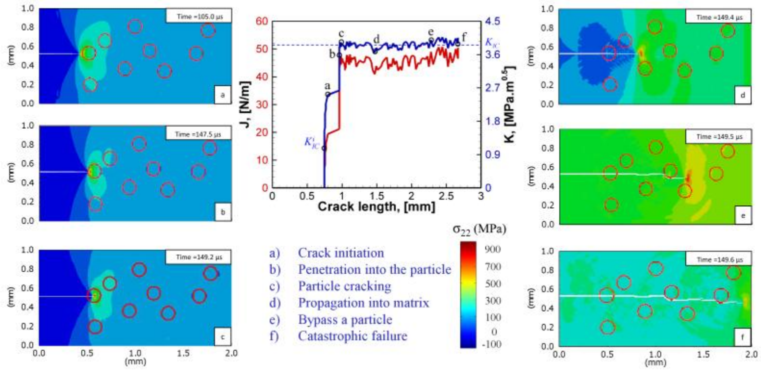


Fig. 2 Crack propagation in a microstructure with circular reinforcement and the evolution of *J* and *K* during this process.

## RESULTS AND DISCUSSION

Calculations carried out concern $Al_2O_3/TiB_2$ two-phase ceramic composites and focus on the fundamental fracture mechanisms during crack initiation and propagation. Results of CFEM calculations show that both microstructure and constituent properties can significantly influence fracture behavior and combine to determine the overall fracture toughness through the activation of different fracture mechanisms. Interface debonding is the most beneficial fracture mechanism and is primarily promoted by small reinforcement size, rounded particle shapes and appropriately bonded and compliant reinforcement-matrix interfaces. In contrast, particle cracking, which triggers catastrophic material failure, usually occurs in microstructure with large reinforcement particles, lower particle roundness and over-bonded/stiff interfaces. Important constituent parameters are the fracture toughness of the matrix phase and the toughness of the interface between the matrix and the reinforcement phases.

## CONCLUSIONS

CFEM calculations show that microstructure and constituent properties can significantly influence fracture behavior. Microstructure size scale refinement, attainment of more rounded reinforcement morphology and appropriately balanced interfacial bonding strength can lead to enhanced material fracture toughness. The CFEM framework is useful tools for the design of failure-resistant materials.

## References

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