Computational Materials Science 116 (2016) 44–51

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

# Prediction of fracture toughness scatter of composite materials

Yan Li [a,*], Min Zhou [b]

[a] Department of Mechanical and Aerospace Engineering, California State University, Long Beach, CA 90840, USA
[b] The George W. Woodruff School of Mechanical Engineering, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405, USA

ARTICLE INFO

*Article history:*
Received 16 July 2015
Received in revised form 26 September 2015
Accepted 28 September 2015
Available online 23 October 2015

*Keywords:*
Fracture toughness
Microstructure
Weibull distribution
Crack deflection/penetration
Two-point correlation functions

ABSTRACT

Fracture toughness of a composite material is not a deterministic property. This is primarily due to the stochastic nature of its microstructure as well as the activation of different fracture mechanisms during the crack-microstructure interactions. Although Weibull distribution has been widely used to determine the probability of material fracture, its role has been confined to fitting fracture toughness data rather than providing predictive insight of material fracture toughness and the magnitude of scatter. Besides, the Weibull parameters which are obtained through curve fitting carry little physical significance. In this paper, an analytical model is developed to predict fracture toughness in a statistical sense. The Weibull distribution parameters are correlated with the statistical measures of microstructure characteristics and the statistical characterization of the competition between crack deflection and crack penetration at matrix/reinforcement interfaces. Although the quantification is specific to $Al_2O_3/TiB_2$ composites, the approach and model developed here can be applied to other materials. The established correlations will lead to more reliable material design.



## 1. Introduction

One of the biggest challenges in material sensitive design is to predict the variation of key material properties such as strength and fracture toughness. It has been proved that the stochastic nature of microstructure is the primary reason for fracture toughness scatter [1–3]. The crack interactions with microstructure can result in different failure mechanisms which ultimately determine the variation of fracture toughness [4,5]. Most of the existing probabilistic models for fracture toughness prediction only consider near crack-tip stress states [6–8]. Information regarding microstructure characteristics and failure mechanisms associated with the crack propagation process is not explicitly included in the model formulations. This is due to the fact that the material heterogeneities at the microstructure level and the interaction of a propagating crack with phases in a microstructure are hard to quantify. Both of them are very random and complicated. Li and Zhou [5] developed a semi-empirical model which allows fracture toughness of $Al_2O_3/TiB_2$ ceramic composites to be predicted. Although this quantification lends itself to the establishment of relations between the statistical attributes of microstructure, fracture mechanism and the fracture toughness of the material, the material fracture toughness is predicted in an average sense from the CFEM (Cohesive Finite Element Method) simulations in Li and Zhou [2]. Based on the previous work, a modified analytical model is introduced which allows the possible range of fracture toughness values to be predicted as function of microstructure. The Weibull distribution parameters are directly correlated to the two-point correlation functions as well as the quantification of fracture mechanisms. These relations can be used for material reliability design by controlling the fracture toughness scatter through microstructure tailoring.

## 2. Determination of fracture mechanism during crack-microstructure interactions

For $Al_2O_3/TiB_2$ ceramic composites, a crack can propagate into $Al_2O_3$ matrix, $TiB_2$ reinforcements or along the interface in between. Our attention is primarily focused on the last two scenarios because they are the two competiting fracture mechanisms when a crack interacts with reinforcements. He and Hutchinson [9,10] first proposed an energy based criterion which quantifies the competition between crack deflection and crack penetration when a semi-infinite crack is perpendicular to an infinite planar interface. This criterion is only valid for isotropic bi-material which is symmetrically loaded. Gupta et al. [11,12] extended He and Hutchinson's work to anisotropic materials and developed a stress based criterion to determine the activation of the two competiting fracture mechanisms. Their results were validated through laser spallation experiments. Later on, Martínez and Gupta [13] further

* Corresponding author.

http://dx.doi.org/10.1016/j.commatsci.2015.09.061
0927-0256/

**Nomenclature**

| | |
|---|---|
| $E_i$ | Young's modulus ($i$ = 0 or 1) |
| $\bar{E}$ | effective Young's modulus of the composite material |
| $f$ | volume fraction of reinforcements |
| $\Phi_m, \Phi_{in}, \Phi_p$ | surface energy of matrix cracking, interface debonding and particle cracking |
| $H_m, H_{in}, H_p$ | fractions of matrix cracking, interface debonding and particle cracking |
| $K_{IC}$ | fracture toughness |
| $K_0$ | normalization factor |
| $m$ | shape parameter |
| $l_m$ , $l_p$ | crack length associated with interface debonding and particle cracking during single crack-particle interaction |
| $\mu_i$ | shear modulus ($i$ = 0 or 1) |
| $P_{ij}$ | two-point correlation functions ($i$ = 0 or 1; $j$ = 0 or 1) |
| $P_f$ | probability of fracture |
| $R$ | particle radius |
| $U$ | parameter in determining the competition between crack deflection and crack penetration |
| $U_f$ | total fracture energy released |
| $\nu_i$ | Poisson's ratio ($i$ = 0 or 1) |
| $\bar{\nu}$ | effective Poisson's ratio of the composite material |
| $\omega$ | crack interaction angle |
| $\omega_0$ | critical crack angle for crack deflection and crack penetration transition |
| $W$ | total projected crack length |

improve the criterion so that both single deflection and double deflection at the interface are considered. This criterion uses quasi-static approximation by assuming crack deflection only occurs under constant loading. Although the above work provides sound theoretical basis for quantifying the competition between crack deflection and crack penetration, these criteria cannot be directly applied to analyze real composite materials. First of all, the reinforcements in real composite materials have finite size. Therefore, the interface cannot be considered as infinite. Besides, it has been proved that the shape of reinforcements also influence the activation of different fracture mechanisms. The shape of reinforcements needs to be quantified and included in the criterion as well.

Based on the previous work, Li and Zhou [5] further extend He and Hutchinson's criterion by including the effects of finite reinforcement size, reinforcement shape and distribution in a two-phase composite material. The criterion is parameterized by

$$U = \frac{1-\beta^2}{a_0(1-\alpha)}\left[|c|^2 + |h|^2 + 2R_e(ch)\right]\bar{\rho}^{a_1} e^{\left(\frac{a_2}{s}\right)} - \frac{\Phi_{in}}{\Phi_p}, \tag{1}$$

to determine the activation of the two competing failure mechanisms. Specifically, interface debonding, which is activated by crack deflection, is predicted when $U > 0$. Otherwise, crack penetration induced reinforcement cracking will be activated instead. In the above relation, $\bar{\rho}$ is the roundness of the reinforcement. $s$ represents the characteristic reinforcement size. $\Phi_{in}$ and $\Phi_p$ are the surface energies of the interface and reinforcement, respectively. For the $Al_2O_3/TiB_2$ ceramic composite material considered in this study, $\Phi_{in}$ and $\Phi_p$ are taken as 78.5 $J/m^2$ and 102.2 $J/m^2$, respectively. Although the surface energy of matrix $\Phi_m$ is not included in Eq. (1), $\Phi_m$ = 21.5 $J/m^2$ is used for the rest of the study. $c$ and $h$ are coefficients which depend on the crack interaction angle $\omega$ as shown in Fig. 1(a). The derivation of $c$ and $h$ as well as other parameters in Eq. (1) are discussed in detail in Li and Zhou [5].

To simplify the problem, we consider circular $TiB_2$ reinforcement particles in the microstructure. $\bar{\rho}$ and $s$ in Eq. (1) are reduced to 1 and 2$R$, respectively. Here, $R$ is the particle radius. Fig. 1(a) illustrates the evolution of $U$ as $\omega$ varies at $R$ = 30 μm. $0 \leqslant \omega \leqslant \pi/2$ is considered in the formulation. $\omega_0$ is defined as the critical crack angle which signifies the transition from crack penetration to crack deflection. Fig. 1(b) compares the $U$ evolution under different particle sizes. It is noted that $\omega = 0^\circ$ is the most difficult scenario for crack deflection. When the crack gradually deviates from the center plane as $\omega$ increases, $U$ increases and create a more favorable condition for crack deflection. It is also observed that the activation of crack deflection is independent of $\omega$ when the particle size is sufficiently small. As shown in Fig. 1(b), the calculated $U$ value from Eq. (1) is always above zero when $R$ = 10 μm. As $R$ increases, $\omega_0$ increases accordingly and creates a more demanding requirement for crack deflection. Therefore, large particle is more susceptible to crack penetration. The conclusions predicted above reflect the trends reported in other studies [4,14,15].

It should be noted that the work above only considers single crack-particle interaction. In real crack propagation problems, the crack can have multiple interactions with the particles, which adds extra complexity to the problem. Even for the single crack-particle interaction, different crack paths are activated as $\omega$ changes. Since the choice of $\omega$ is random, the prediction of upper bound and lower bound of fracture toughness needs to consider all the possible $\omega$ values. As shown in Fig. 2, $l_{in}$ and $l_p$ represent the crack length for interface debonding and particle cracking under single crack-particle interaction, respectively. $l_{in}$ and $l_p$ are calculated as

$$\begin{cases} l_{in} = (\pi - 2\omega)R, & \text{if } \; U > 0, \\ l_p = 2R\cos(\omega), & \text{if } U \leqslant 0. \end{cases} \tag{2}$$

As illustrated in Fig. 2, interface debonding is the only fracture mechanism being activated when $R$ = 10 μm. The maximum crack length is reached at $\omega = 0^\circ$. The same trend is observed when $R$ = 200 μm with particle cracking as the only failure mechanism. The above scenarios represent two extreme cases when the particle size is either very small or very large. When the particle size is in between (for example, when $R$ = 20 μm and 30 μm), the maximum crack length is obtained at $\omega_0$ which is also the point where a fracture mode changes from interface debonding to particle cracking.

As discussed earlier, Eq. (2) only applies to single crack-particle interaction. For multiple crack-particle interactions, it is necessary to statistically parameterize the probability of crack encounter with the particle phase. In this paper, two-point correlation functions are employed for this task. The purpose of using two-point correlation functions is two-fold. First of all, these functions have been proved to be effective for microstructure characterization and generation [2,16,17]. Mathematically, the four two-point correlation functions $P_{ij}$ $(i,j = 0 \text{ or } 1)$ measure the probability of finding a given combination of phases over given distance. Since $P_{00} + P_{01} + P_{10} + P_{11} = 1$, only three of the four two-point correlation functions are independent. For example, $P_{11}$ quantifies the probability to randomly locate both the starting point and ending point in phase 1. It is a function of $D$ which is the distance between the two points. In this study, phase 0 and phase 1 represent matrix and reinforcement, respectively. It can be inferred that both the starting point and ending point will overlap with each other when $D = 0$. $P_{11}$ at $D = 0$ is equivalent to the probability of finding the reinforcement phase over the entire microstructure region, which is actually the volume fraction $f$ as shown in Fig. 3. When $D \to \infty$, the starting point and ending points are not correlated any more.