

# Influence of interfacial microcracks on the elastic properties of composites

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A model is established to quantify the influence of interfacial microcracks on the elastic properties of a particulate composite using a combination of theoretical and finite element analysis. A unique way to construct physical models which could accommodate both crack size and crack density is proposed. Based on energy principles, the influence of a dilute concentration of interfacial microcracks is first studied. The case of a finite concentration of microcracks is solved subsequently by combining the dilute concentration solutions and the differential scheme. Both cases agreed well with existing composite theories for the limiting condition of complete decohesion. The final model predicts the effective elastic properties as functions of both crack size and microcrack density.

## 1. Introduction

Microcracking can occur in ceramic matrix composites due to applied or residual stresses. These localized stresses usually arise from the differences in elastic modulus or thermal expansion of the constituent materials. In general, the formation of microcracks damages the integrity of the material, and thus degradation in properties, such as strength and stiffness, is inevitable. Therefore, for the purposes of engineering design and tailoring composite properties, it is desirable to establish the relationship between degree of microcracking and composites performance.

The determination of the effective elastic properties of cracked materials has attracted substantial attention in the fields of both mechanics and materials in the past decade. Since Budiansky and O'Connell [1] first presented their classic paper on this topic in 1976, numerous variations and approaches have been attempted [2–11]. A comprehensive review on the microcracking of monolithic materials has been given by Kachanov [12]. Despite the numerous studies on this topic, however, analysis of the effective properties of microcracked *composites* are still relatively rare in the literature, and most of them pertain to fibre composites. Even fewer studies are found on the effect of a partially debonded fibre matrix interface on the composite elastic properties [11, 13–15]. Studies on the reduction of stiffness due to partially debonded spherical particle/matrix interfaces, to the authors' knowledge, do not exist. Apparently, if one wishes to assess the integrity of composite materials by evaluation of the elastic properties, a new model needs to be developed. The common feature of the above-mentioned analyses, however, is the extremely com-

plex, and sometimes intractable, mathematical expressions. Therefore, further exploration or development of similar mathematical treatments was discounted. Instead, a numerical approach, namely finite element analysis, was adopted to establish a new model.

The specific objective of this study was to quantify the reduction of elastic modulus of an interfacially microcracked composite, namely Hexoloy ST\*, a 15 vol % TiB<sub>2</sub> particulate reinforced SiC. As the thermal expansion coefficient of TiB<sub>2</sub> is larger than that of SiC, this composite tends to form interfacial microcracks as a result of the tensile residual stress acting radially across the interface. Previous studies [16, 17] have shown that Hexoloy ST contains microcracks at the TiB<sub>2</sub>/SiC interface and these cracks will influence mechanical properties. For convenience, the TiB<sub>2</sub> particulates will be treated as spherical particles and all the constituent materials are considered isotropic.

## 2. The approach

### 2.1. The constituents

An interfacially microcracked composite is considered to be composed of two constituents: the "composite spheres" and the "effective medium." Both constituents contain the same concentration of TiB<sub>2</sub> particles. The composite sphere is composed of a TiB<sub>2</sub> sphere and a concentric SiC layer, with an interfacial microcrack of size  $\phi$  (Fig. 1). The radii  $a$  and  $b$  are related to the volume fractions of TiB<sub>2</sub> and SiC. On the other hand, the effective medium is a homogenized medium that possesses the properties of a non-microcracked composite.

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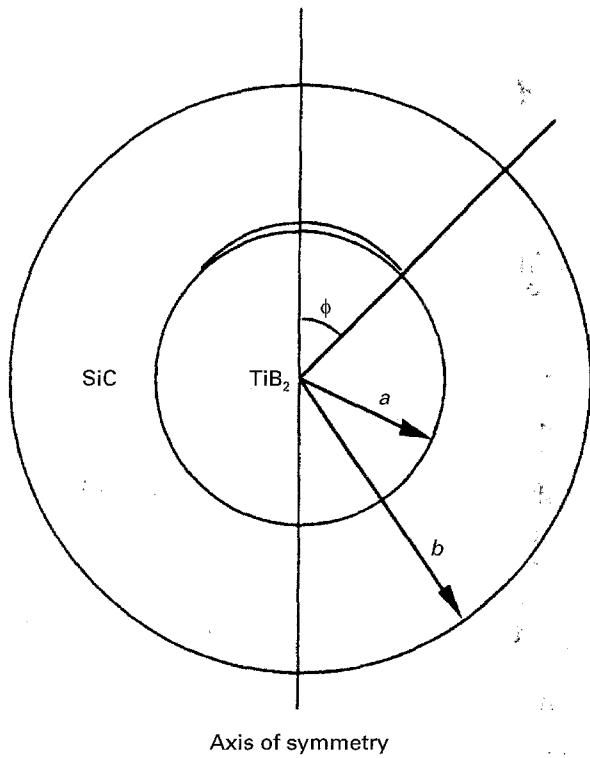


Figure 1 Schematic of the composite sphere which contains an interfacial microcrack.

A microcracked composite is built up by adding composite spheres into the effective medium. As both constituents have the same  $\text{TiB}_2$  concentration, the volume fraction of the composite sphere represents the fraction of interfacially microcracked  $\text{TiB}_2$  particles in the overall  $\text{TiB}_2$  population. This fraction will be called the “debonded fraction” and denoted by  $f$  in the following text. Thus, with this physical model, both the size of the microcracks and the debonded fraction are considered.

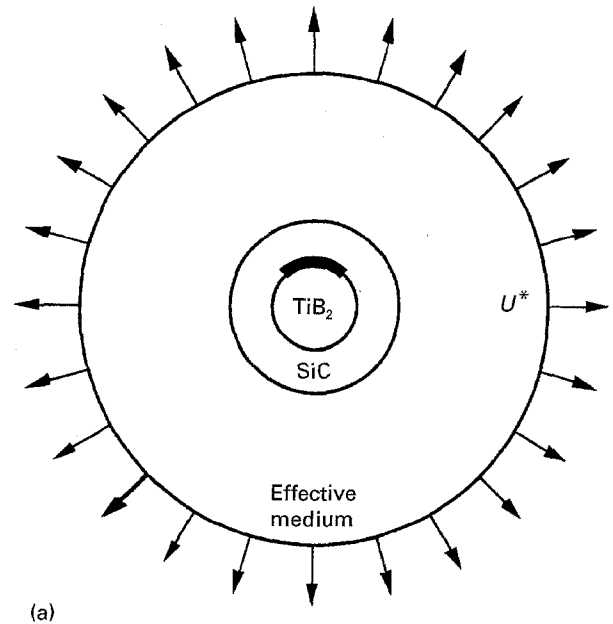
## 2.2. Dilute concentration

Consider the two models in Fig. 2. One model (microcracked) is composed of one composite sphere and the effective medium, while the other (non-microcracked) contains only the effective medium. When the models are subjected to the same stresses, the stored elastic strain energy in the microcracked model is less than that in the non-microcracked model due to the presence of the microcrack. The strain energies in the microcracked and non-microcracked models are denoted as  $U^*$  and  $U_0$ , respectively, and they are related by:

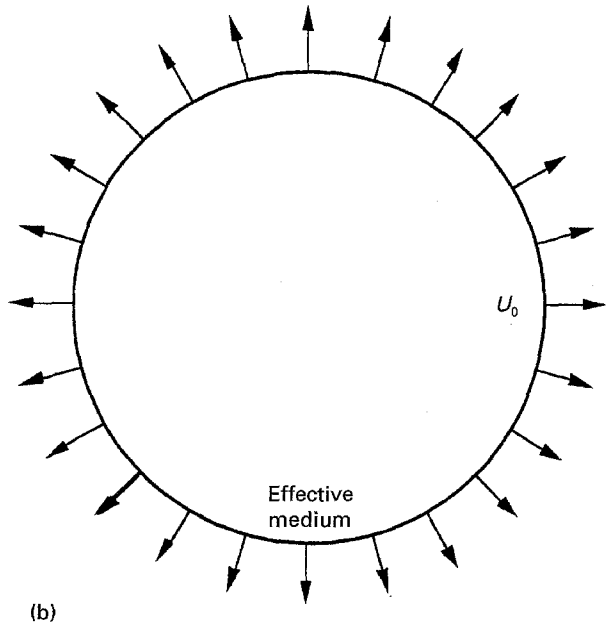
$$U^* = U_0 - \Delta U \quad (1)$$

The difference,  $\Delta U$ , is the disturbance in strain energy due to the presence of the composite sphere. The disturbance can be normalized by the volume of the composite sphere:

$$\Delta u = \frac{\Delta U}{\frac{4}{3}\pi b^3} \quad (2)$$



(a)



(b)

Figure 2 (a) A model composed of one composite sphere and the effective medium. (b) A model composed of only the effective medium.

where  $\Delta u$  is the disturbance in strain energy caused by one unit volume of composite sphere, or the “disturbance density.”

When more composite spheres are added, the total strain energy disturbance changes. If only a dilute concentration of composite spheres is added, i.e., no interactions among the composite spheres, the total strain energy disturbance is the summation of individual disturbances. Assume that there are  $m$  composite spheres of crack size  $\phi$  evenly distributed and randomly oriented in the effective medium (Fig. 3), the difference between the microcracked model and the non-microcracked model can be written as:

$$\sum_{m=1}^m \Delta U_m = m \frac{4}{3}\pi \langle b^3 \rangle \Delta u \quad (3)$$

where the angle brackets,  $\langle \rangle$ , are used to represent an average value.

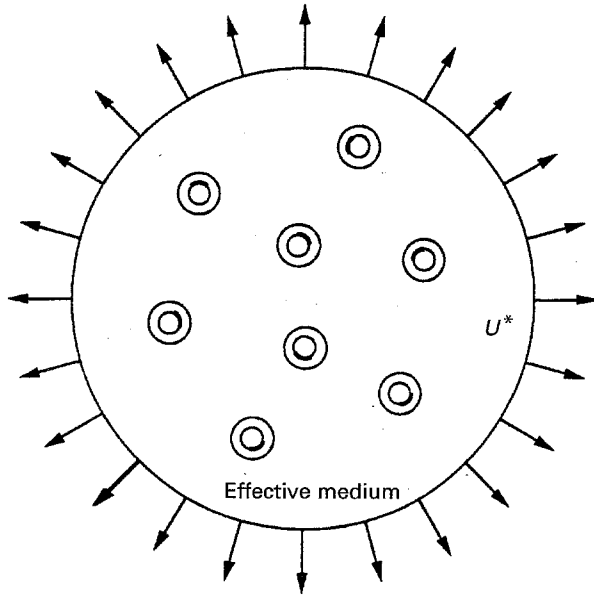


Figure 3 A model composed of multiple composite spheres and the effective medium.

Assume that identical hydrostatic displacements are applied to the two models, shown in Figs 2b and 3. The corresponding applied strain is  $\varepsilon_0$ . If the volume of the model is  $V$  and there are  $m$  composite spheres in the microcracked model, the relationship between the two models can be expressed by

$$U^* = U_0 - \sum_{m} \Delta U_m \quad (4)$$

Rewriting Equation 4 in terms of strain and bulk modulus gives:

$$\frac{9}{2} K^* \varepsilon_0^2 V = \frac{9}{2} K_0 \varepsilon_0^2 V - \sum_{m} \Delta U_m \quad (5)$$

which yields

$$K^* = K_0 - \frac{2}{9} \frac{1}{\varepsilon_0^2} \frac{1}{V} \sum_{m} \Delta U_m \quad (6)$$

where  $K_0$  is the bulk modulus of the effective medium and  $K^*$  is the bulk modulus of the microcracked composite. Equation 6, however, has to be transformed further into an expression dependent on the concentration of the composite spheres. To do so, the last term of Equation 6 can be rearranged:

$$\frac{1}{V} \sum_{m} \Delta U_m = \frac{\frac{4\pi}{3} m \langle b^3 \rangle}{V} \cdot \frac{\sum_{m} \Delta U_m}{\frac{4\pi}{3} m \langle b^3 \rangle} = f \Delta u \quad (7)$$

where  $f$  is the "debonded fraction," as defined in Section 2.1. Therefore, the bulk modulus of the microcracked composite is:

$$K^* = K_0 - \frac{2}{9} \frac{1}{\varepsilon_0^2} \Delta u f. \quad (8a)$$

A similar result can be derived for the effective shear modulus:

$$G^* = G_0 - \frac{2}{9} \frac{1}{\varepsilon_0^2} \Delta u' f. \quad (8b)$$

where  $G^*$  is the effective shear modulus,  $G_0$  is the shear modulus of the effective medium, and  $\Delta u'$  is the strain energy disturbance caused by an applied shear strain.

Note that the only unknown variable in Equation 8 is  $\Delta u$ , the disturbance density. Therefore, the key to the problem indeed relies on the determination of the strain energy disturbance in the presence of *one* composite sphere. Because of the complex elastic field near an interfacial microcrack, the strain energy has to be determined numerically.

### 2.3. Finite concentration

For the case of a finite concentration of composite spheres, the interaction among spheres has to be approximated. After reviewing the existing modelling schemes, the differential scheme was adopted for this approximation. The basis idea in this approach is to consider the construction of a composite as a sequence of operations involving only dilute concentrations of composite spheres [18]. As illustrated in Fig. 4, a dilute concentration of composite spheres is first added to the effective medium, and then this composite is "homogenized," or recognized as a new (microcracked) "effective medium." Similar operations can subsequently be performed on this effective medium until a finite concentration is achieved.

As the differential scheme involves only a dilute concentration of composite spheres in each step of the calculations, the previous method for dilute concentrations is still applicable. However, an important issue arises from the adoption of the differential scheme: the properties of the homogeneous media are constantly changing during the iterations. As a result, the dilute concentration analysis, which only dealt with the effective medium, has to be modified to accommodate the changing properties of the homogeneous media.

For each step, it was assumed that the effective bulk modulus of a composite is independent of the shear modulus of the homogeneous medium. It was further assumed that, when a dilute concentration ( $f \ll 1$ ) of composite spheres is added into *any* homogeneous medium, the effective bulk modulus ( $K^*$ ) of that composite can be written as:

$$K^* = K_{HM} + (A - BK_{HM})f \quad (9)$$

where  $K_{HM}$  is the bulk modulus of the homogeneous medium, and  $A$  and  $B$  are constants to be determined. The form of Equation 9 was chosen to mimic the universal expression given by Hill [19]:

$$M^* = M_1 + (M_2 - M_1) \frac{\bar{\varepsilon}^{(2)}}{\bar{\varepsilon}} c_2 \quad (10)$$

where  $M$  is the stiffness tensor, subscripts 1 and 2 denote the phases,  $\bar{\varepsilon}^{(2)}$  is the average strain in phase 2,  $\bar{\varepsilon}$  is the homogeneous boundary condition, and  $c$  is the volume fraction. Obviously, the constants  $A$  and  $B$  are thus, to some extent, implicit expressions of the complex terms that are used in solutions with the form shown in Equation 10. In order to obtain the values of

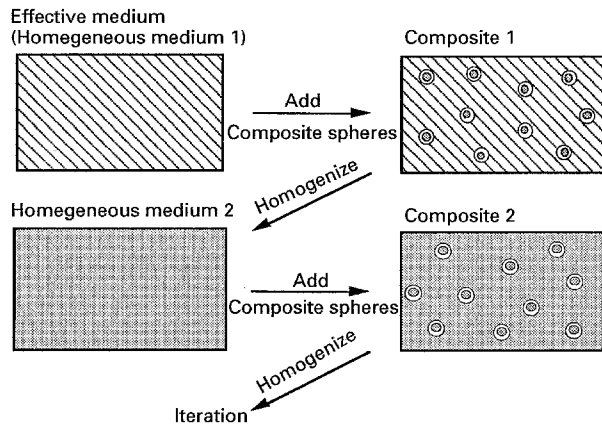


Figure 4 Schematic illustrating the steps in the differential scheme approach.

$A$  and  $B$ , the operations shown in the previous section were repeated for various bulk moduli of the homogeneous media. The results were then fitted to Equation 9 using linear regression to determine  $A$  and  $B$ . As it turned out, the above two assumptions were reasonable, as the linear regression always leads to a coefficient of determination ( $r^2$ ) of value 1.000, indicating an excellent fit.

When the composite spheres are gradually added into the homogeneous media, extreme care has to be taken in adjusting the relative concentration of the constituents. Proper formulation of the differential scheme [20] would give a governing equation for any finite concentration of composite spheres in the form:

$$\frac{dK^*}{df} = \frac{1}{1-f}(A - BK^*) \quad (11)$$

where  $K^*$  is the effective bulk modulus of the composite.

This ordinary differential equation can be solved easily. The effective bulk modulus of a composite containing a finite concentration of composite spheres is therefore:

$$K^*(f) = \frac{A}{B} + \left(K_0 - \frac{A}{B}\right)(1-f)^B \quad (12)$$

where  $K_0$  is the bulk modulus of the starting effective medium.

## 2.4. The finite element analysis

Finite element analysis was adopted for the calculation of strain energy. A commercial package ANSYS<sup>†</sup> was used. The cross-sections of the two models shown in Fig. 2 were built using element type STIF 83, an 8-node axisymmetric structural solid. The meshes, which were generated automatically using the ANSYS built-in algorithm, were almost identical except for the difference in separation at the interface. Special control was taken near the crack front, where large stress gradient exists, to minimize the computational error.

TABLE I The elastic properties used in this study (GPa). Note that they are extrapolated values for fully dense materials [20]

Material	Young's modulus	Shear modulus	Bulk modulus
SiC	430.2	191.1	191.5
TiB <sub>2</sub>	568.8	259.5	234.6
Hexoloy ST	414.4	186.7	177.5
Effective medium <sup>†</sup>	448.6	200.0	197.5

<sup>†</sup> Estimated based on self-consistent scheme for a 15 vol % composite [21].

In this study, calculations were performed only for the effective bulk modulus. The elastic fields within a model were first determined, and then the total elastic strain energy was tallied for the body of revolution based on the cross-section. As Hexoloy ST is the candidate composite that contains microcracks, the calculations were performed for 15 vol % TiB<sub>2</sub> particulate reinforced SiC. The properties of the constituent materials are summarized in Table 1, where the properties of the effective medium were calculated by using the self-consistent scheme [21].

## 3. Results and discussion

### 3.1. Dilute concentration

The calculated results were first compared to existing solutions to verify their validity. The only available case, however, is the extreme condition that the crack size ( $\phi$ ) is 180°, i.e., the TiB<sub>2</sub> particles are totally debonded from the SiC matrix. For convenience, the totally debonded TiB<sub>2</sub> particles are treated as pores. In other words, a composite is considered as a three-phase composite: porosity, TiB<sub>2</sub> particles, and SiC matrix. Subsequently, the elastic properties of this three-phase composite could be predicted using conventional models such as the self-consistent scheme [21].

Assume that 1 vol % of the TiB<sub>2</sub> particles are totally debonded. Therefore, an original 15 vol % TiB<sub>2</sub> composite is composed of 0.15 vol % porosity, 14.85 vol % TiB<sub>2</sub> particles, and 85 vol % SiC as a matrix. The present model predicts a reduction in bulk modulus of 0.577 GPa when compared to a non-microcracked composite. The self-consistent scheme gives a reduction of 0.581 GPa. Alternatively, one can consider the influence of the 0.15 vol % porosity in a composite which has a TiB<sub>2</sub>:SiC ratio of 14.85:85. To do this, the modulus of the latter composite was first calculated using the self-consistent scheme, and then the influence of porosity was accounted for by using the exact solution for dilute concentration of second phase given by Hashin [22]. Such an approach yielded a modulus reduction of 0.568 GPa. It is significant to find that the dilute concentration model provides an excellent prediction, which differs less than 2% from the conventional predictions, thereby

<sup>†</sup> ANSYS version 4.4a, Swanson Analysis Systems, Houston, PA

corroborating the validity of the dilute concentration model.

For clarity, Equation 8a is rewritten in the following form:

$$K^* = K_0 - Df \quad (13)$$

where

$$D = \frac{2}{9} \frac{1}{\varepsilon_0^2} \Delta u$$

The coefficient  $D$  is plotted as a function of crack size ( $\phi$ ) in Fig. 5. This shows that as a crack grows, it becomes more effective in reducing the stiffness of the composite. At small crack sizes, the reduction rate ( $D/\phi$ ) is low. As the crack propagates along the interface, the debonded area increases rapidly, which corresponds to the increased reduction rate. Finally, the reduction rate decreases and the crack totally separates the TiB<sub>2</sub>/SiC interface for  $\phi = 180^\circ$ . Although the behaviour shown in Fig. 5 is intuitively expected, this is the first time that such a relationship has been shown quantitatively.

### 3.2. Finite concentration

The constants  $A$  and  $B$ , determined, from the finite element analysis, are listed in Table II. Substituting these values into Equation 12, the effective bulk modulus can be written as a simple function of the TiB<sub>2</sub> debonded fraction ( $f$ ). The effective bulk modulus of a 15 vol % composite is plotted as a function of debonded fraction for various crack sizes (Fig. 6). The effective modulus shows a rather linear dependence on the TiB<sub>2</sub> debonded fraction.

Similar to the previous section, the results of the finite concentration model were compared to limiting cases to verify the validity of the model. It was assumed that the crack size is  $180^\circ$  and the debonded fraction is 100%, i.e., all TiB<sub>2</sub> particles are totally debonded. Therefore, the composite was composed of 15 vol % porosity and 85 vol % SiC. The self-consistent scheme predicts an effective bulk modulus of 140.6 GPa. On the other hand, the Hashin–Shtrikman upper bound [21] predicts 150.3 GPa. Note that in the presence of pores, the Hashin–Shtrikman lower bound vanishes as it implies the material becomes incoherent. The current finite concentration model predicts an effective bulk modulus of 149.1 GPa, which is in good agreement with both theoretical predictions. In particular, the close results of this model and the Hashin–Shtrikman upper bound are desired, as these two models have very close resemblance in physical geometry.

### 3.3. Implications

The above results provide an insight on the microcrack density in Hexoloy ST. For example, if all microcracks are  $60^\circ$ , the bulk modulus of a totally microcracked 15 vol % composite is 183.2 GPa. As the measured bulk modulus of Hexoloy ST was 177.5 GPa [20], the results imply that some micro-

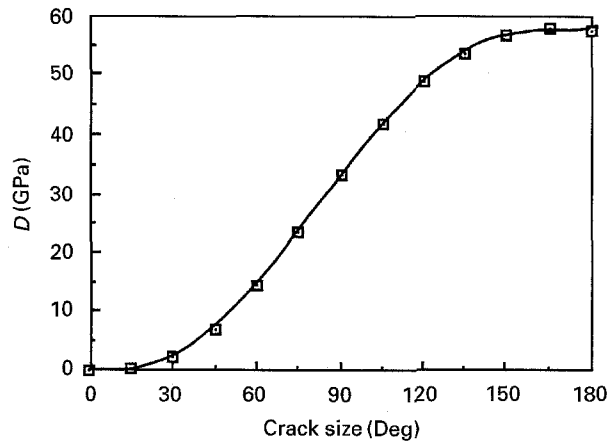


Figure 5 The influence of different crack size ( $\phi$ ) on the reduction of bulk modulus at dilute concentration. See Equation 13 for the definition of  $D$ .

TABLE II The constants  $A$  and  $B$  determined from the finite element analysis. See Section 2.3 for the definitions of  $A$  and  $B$

Crack size	$A$ (GPa)	$B$
$30^\circ$	186.6	0.9560
$60^\circ$	183.7	1.003
$90^\circ$	180.8	1.082
$120^\circ$	178.2	1.149
$150^\circ$	177.3	1.183
$180^\circ$	176.7	1.185

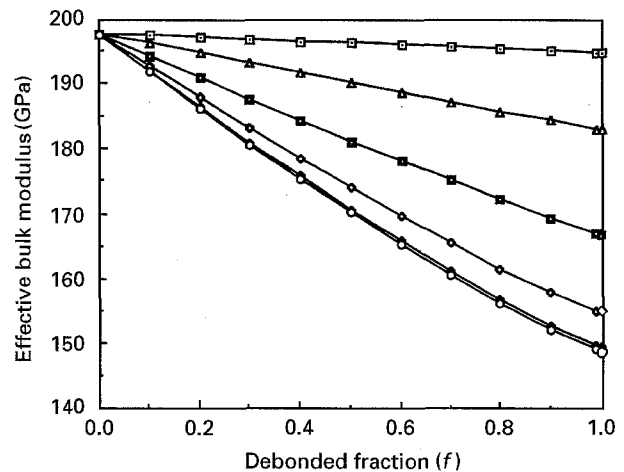


Figure 6 The effective bulk modulus of an interfacially microcracked composite plotted as a function of debonded fraction (microcrack density) for various crack sizes. The data is for microcrack sizes of; (□)  $30^\circ$ , (△)  $60^\circ$ , (■)  $90^\circ$ , (◇)  $120^\circ$ , (◆)  $150^\circ$  and (○)  $180^\circ$ .

cracks must be larger than  $60^\circ$ . On the other hand, if all microcracks are  $90^\circ$ , Fig. 6 predicts that 63 vol % of TiB<sub>2</sub> are debonded.

One major difficulty encountered in the above assessment is the determination of actual crack size. As the average TiB<sub>2</sub> particle size in Hexoloy ST is approximately 5  $\mu\text{m}$ , the only viable way to observe microcracks is conducting transmission electron microscopy (TEM). However, TEM observations would not provide any quantitative information regarding crack size because the observed image could

be any cross-section of a particle, not to mention the possible damage to the composite during sample preparation. Therefore further verification of the model has to be performed on other composite systems where crack size can be easily determined.

Clearly, the microcracks in a real composite are not necessarily of a single size. If one can define the crack size distribution, the analyses in the previous sections can easily be extended to contain multiple crack sizes. Once the disturbance densities ( $\Delta u$ ) of different crack sizes are calculated, the effective bulk modulus ( $K^*$ ) can be determined by:

$$K^* = K_0 - \frac{2}{9} \frac{1}{\varepsilon_0^2} (\Delta u_{\phi_1} V_{\phi_1} + \Delta u_{\phi_2} V_{\phi_2} + \dots) f \quad (14)$$

where the subscripts  $\phi_1$ ,  $\phi_2$ , and so on, denote different crack sizes, and  $V$  is the fraction of a particular crack size in the overall composite sphere population. Subsequently, the influence of these cracks at finite concentration can be quantified by following the analysis presented.

#### 4. Conclusions

A model is established to quantify the influence of interfacial microcracks on the elastic properties of a composite using a combination of theoretical study and finite element analysis. A unique way to construct physical models which could accommodate both crack size and crack density was proposed. The case of a dilute concentration of microcracks was solved and subsequently extended to the case of finite concentration by adapting the differential scheme. Both cases agreed well with existing composite theories for the limiting condition of complete decohesion. The influence of crack size and crack density on the reduction of effective modulus were examined. In particular, for 15 vol %  $\text{TiB}_2$  particulate reinforced SiC composites, the effective modulus showed a rather linear dependence on the  $\text{TiB}_2$  debonded fraction (crack density).

With this model, not only can one accurately predict the elastic properties of an interfacially microcracked composite, but also one can use the model to assess the severity of microcracking from measured elastic properties. Above all, the straightforward approach provides a convenient way to construct the

property-microstructure relationship for other composite systems.

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