Geometrical factors related to composite microcracking

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With the addition of second-phase reinforcements to a monolithic matrix it is possible to create structural systems from materials that are normally considered unsuitably weak or brittle. For example, the addition of a soft, ductile phase to a hard, brittle matrix can significantly increase the toughness and possibly the failure strain of the brittle component. However, due to the variation of processing techniques, the second-phase reinforcements can be formed into either elongated strands or more equiaxed dispersoids resulting in a range of fracture properties for a given material combination. The finite element analysis presented here quantifies the plane-strain elastic interaction between a crack under pure mode I loading and a particle in terms of crack length, particle size, particle shape and crack-particle separation. Findings suggest that the influence of a particle on a crack tip decreases rapidly as the crack-particle distance increases so that an effective zone can be defined around the particles in which the particles directly affect crack propagation. Outside of this zone, cracks do not interact elastically with particles to any significant extent. The size of the zone is a function of crack length and particle size. In the specific case of NiAl reinforced with Nb, the zone width is approximated to be on the order of the grain size. For all reasonable values of Dundurs' parameters, α and β, shape-specific relations are given for a wide range of specimen geometries in order to provide simple, yet accurate estimates of the stress intensity factors of cracks in the composite. For the case of plastically deforming inclusions, the analysis becomes more complicated due to the introduction of the non-linear relationship between stress and strain, as well as the variable yield stress and strain hardening exponent.

1. Introduction

Composite materials are increasing in prominence in structural applications as advances in mechanical properties such as strength and toughness exceed those of conventional materials. These composites are based on combinations of metals, polymers and ceramics with a wide range of phase volume fractions and arrangements. Two specific examples of this extremely broad class of materials are Al–SiC and Al₂O₃–SiC which demonstrate toughness, strength, thermal shock and creep resistance superior to the unreinforced materials [1–4]. Conversely, the introduction of inhomogeneities in a matrix can lead to the degradation of mechanical properties due to inappropriate phase distribution and low interfacial bond strength or secondary chemical reactions and residual stresses. A combination of certain materials may therefore succeed or fail as a potential structural composite from factors related to processing in addition to the more fundamental properties of the components such as thermal expansion characteristics or strength.

It is difficult if not impossible to predict exactly how any two or more materials will behave when combined, although researchers are making advanced models for certain aspects of deformation and failure [5–12]. In the case of composite crack analysis the general approach has been to examine either a single crack and circular particle in an infinite matrix or a crack near an interface [5,13,14]. For a more accurate analysis of cracking in actual materials, the current work considers cracks of various lengths near particles of non-circular shape, with an arbitrary area and elastic modulus. These results are intended to advance the understanding of composite failure.
2. Method

The plane-strain problem that is of interest in this investigation is the influence of the elastic constants and shapes of a particle on the crack-tip stress intensity factor. The model is approached through finite element (FE) calculations using PERMAS with plane-strain elements of the type 6-noded triangles and 8-noded quadrilaterals [15]. A representative schematic of the side-cracked sample geometry is shown in fig. 1 along with the respective boundary conditions. The upper and lower boundaries of the specimen are given equal and opposite displacements in the y-direction, while the other faces are stress-free. The specimen is subjected to these displacements and no thermal or residual stresses are considered at this time. All calculations are based on the assumption that stresses remain within the elastic range of both the matrix and the inclusion.

Two possible specimen geometries are used in this investigation. Calculations are performed for cracks of various lengths situated a fixed distance from an inclusion (variable $a$, fixed $d$) or for a fixed crack length with a variable crack-particle spacing as shown in fig. 2. This combination of calculations systematically characterizes the influence of both variables $a$ and $d$ on the crack tip–particle interaction. The other important features of this specimen geometry pertain to the particle dimensions. Particles of various cross-sectional areas are considered with a variety of shapes, or aspect ratios. The aspect ratio is defined as the dimension of the rectangular particle in the crack plane, divided by the particle height, $w/h$. Aspect ratios here ranged from $\sim 0.05–10$. Under this definition, an aspect ratio of 1 applies to a square, but a circle with an equivalent area was also considered in order to compare these results with results of other authors.

3. Results

The results for the material model described above are plotted on figs. 3 and 4 under the general format of crack-tip stress intensity factor information on the vertical axis and a geometrical parameter on the horizontal axis. Specifically, the figures show $\Delta K/K_H$ values on the ordinate with corresponding $d/a$ values on the abscissa. The differential stress intensity, $\Delta K$, is defined as...
almost no additional changes. The Poisson ratio of 0.3 was used in all calculations for both the matrix and inclusion because it was seen that a range of $\nu$ values for both the matrix and inclusion between 0.2 and 0.4 had an insignificant effect on $\Delta K$.

Figure 3(a) summarizes the results of calculations for constant $d$ (0.8 mm) with various particle aspect ratios, $w/h$, and crack lengths, $a$, for a composite with matrix properties of $E_m = 210$ GPa, $\nu_m = 0.3$ and inclusion properties $E_i = 100$ GPa, $\nu_i = 0.3$. The curves exhibit a maximum for small values of $d/a$ with $\Delta K/K_H$ values that vanish for more extreme values of $d/a$. The most extreme peak height corresponds to the aspect ratio 0.31, but is still relatively low at a $\Delta K/K_H$ value near 5%. Figure 3(b) shows the results for the same calculation with a circular inclusion superimposed over the results for a square. For both a circular and a square inclusion the aspect ratios are one and the areas are equal to 0.8 mm$^2$, but there are obvious differences in geometry. The same general trends shown in fig. 3(a) remain in fig. 3(b), although the peak height for the circular inclusion is roughly double the peak height for the $w/h = 1.25$ values shown in fig. 3(a), and 30% higher than for a square. A larger peak height is expected for a circle because of the higher curvature of the particle-matrix interface in the crack plane.

Figure 4 summarizes the results of a similar series of calculations based on the alternate specimen geometry with varying crack–particle distance. For the data plotted in fig. 4, the particles have the same area and aspect ratios as above, but the crack length is kept constant ($a = 0.8$ mm) and $d$ is variable. For clarity only a limited number of aspect ratio data are plotted but all data show similar trends. In this case, no maximum exists and again the general shape of the curves could be anticipated from the extreme values of $d/a$. When $d$ is large, the inclusion is too distant to affect the crack-tip stress field, thus $\Delta K \ll K_H$. The particle only begins to have a significant influence when $d \leq a$. With a small $d$, the effects of the particle become large because of the proximity of the inclusion in the crack tip. In the effective $d/a$ range ($\leq 1$) the particles
with a higher aspect ratio (elongated in the direction of the crack) produce a greater $\Delta K/K_H$ (over 20%) than the particles elongated perpendicular to the crack. For example, at a $d/a$ value of 0.15, the $\Delta K/K_H$ values for the various shapes can range from 17 to 27%.

4. Discussion

4.1. Shape Influence

A significant difference in the crack-particle interaction exists between specimens with different particle aspect ratios and crack-particle geometries given other identical parameters. In fig. 3 the $\Delta K/K_H$ results for a specimen with a constant $d$ and variable $a$ are plotted for various $w/h$ values. The nature of these curves is understandable in terms of the stress and displacement fields near the crack tip and inclusion, which are comparable in magnitude and in interactive contact only for values of $d = a$ ($\approx 0.8\ \text{mm}$). For more extreme values of $d$ and $a$, the enhanced displacements due to the inclusion or the crack tip are either too distant to interact, or too unevenly matched in magnitude to affect the other to any significant extent. The maximum value of $\Delta K/K_H$ is the point where the interaction is most extensive. The value of $d/a$ corresponding to this peak is $\approx d/w$ which implies that at $a = w$ interaction is most extensive. This maximum is most likely related to the interaction between the regions of increased tensile stress that necessarily exist around the crack tip and soft particle.

Changing the specimen geometry variable to $d$ reveals trends in $\Delta K/K_H$ that are different from those shown above for identical values of $w/h$ with variable $a$. For example, the curves in fig. 4 exhibit the same tendency to approach zero for large $x$-values, although for small $x$-values the trend is reversed. Whereas the curves in fig. 3 decrease at low abscissa values, the curves of fig. 4 continue to increase because the weaker component in close proximity to the crack tip increases the stress on the remaining matrix ligament between the crack tip and the particle.

Figures 3 and 4 show different trends and values of $\Delta K/K_H$ for identical $x$-values therefore a more comprehensive and unique geometrical parameter must be utilized for the $x$-axis. For this purpose a new factor is now introduced into the analysis in order to bring the magnitudes of $d$ and $a$ into consideration rather than simply their ratio. Figure 5 shows the previous $\Delta K/K_H$ values now plotted as a function of

\[
\left[ \frac{d}{a} \left( \frac{d + a}{\sqrt{A}} \right) \right]^{1/2},
\]

where $A$ is the area of the inclusion and $a$ and $d$ have their previous meanings. The trends of the data from figs. 3 and 4 when replotted as on fig. 5 are now in agreement and the differences decrease significantly over the entire abscissa range. A simple expression describing the data shown on fig. 5 in terms of general $x$- and $y$-axes can be written as

\[
y = -31.2x - 33.5 \quad (1)
\]

for abscissa values between 0.3 and 1.0 for all data with an unspecified aspect ratio. For abscissa values greater than 1.0, ordinate values are a constant $\approx 3\%$. Analyzing the relation between $\Delta K/K_H$ and $[(d/a)(d + a)(1/\sqrt{A})]^{1/2}$ indicates that given a constant $a$, the influence of a particle on the crack tip logically decreases as $d$ increases to a point where $\Delta K/K_H$ is insensitive to changes in $d(x > 1)$. Similarly for the constant $d$ and $A$ used here, the particle influence remains small in spite of an increasing $a$ because $[(d/a)(d + a)(1/\sqrt{A})]^{1/2}$ approaches $[d/\sqrt{A}]^{1/2}$ as $a$ increases. The variation in the $\Delta K/K_H$ values for a given abscissa value is due to the aspect ratio effects. More specific relations are written for the various aspect ratios as

\[
\frac{\Delta K}{K_H}[\%] = U \left[ \frac{w}{h} \right] x + V \left[ \frac{w}{h} \right],
\]

where

\[
U \left[ \frac{w}{h} \right] = 3.98 \left[ \frac{w}{h} \right] - 37.3, \quad (3)
\]

\[
V \left[ \frac{w}{h} \right] = -4.64 \left[ \frac{w}{h} \right] + 40.7 \quad (4)
\]

for $0.3 \leq x \leq 1.0$ and $0.3 \leq w/h \leq 3$. 
With the more consistent method of plotting results for different crack-particle geometries and inclusion aspect ratios shown in fig. 5, it must be verified that changing \(d\), \(a\) or \(A\) would result in a \(\Delta K / K_H\) value that conforms to the other data. For a particle area of 0.8 mm\(^2\) the \(d/a\) values of 1.6/2.3 and 1.1/1.6 yield values of \(\Delta K / K_H = 0.9\%\) and 1.7\%, respectively, which are in good agreement with the data plotted in fig. 5. Similarly, the \(d\) and \(a\) values of 0.8 mm and 1.3 mm, respectively, combined with a fourfold increase in particle area (3.2 mm\(^2\)) yields a \(\Delta K / K_H\) value of 8\% for a \([d/a](d + a)(1 / \sqrt{A})]^{1/2}\) value of 0.85. This value is also plotted on fig. 5 and shows good agreement with the other data. With this consistency now confirmed it is possible to estimate values of \(\Delta K / K_H\) for a given \(d\), \(a\) and \(A\) for this combination of material parameters based on eq. (2). Previous authors have investigated internal crack-particle interactions for a circular inclusion but normalized the crack length and crack-particle distance with the radius of a circular particle, which was specified as a constant [5,14]. The current work was the advantage of including particle shape and areas as factors in \(\Delta K / K_H\) calculations. Closer inspection of fig. 5 shows that changing the shape of an inclusion affects the \(\Delta K / K_H\) values as does various \(d\) and \(a\) values. For example, at an abcissa value of 0.53 the different aspect ratio particles yield \(\Delta K\) effects that are roughly a factor of 2 different (11\%-19\%). The coefficients in eq. (2) are functions of \(w/h\) and predicted values are very nearly equal to the results from the various \(w/h\) values. Specifically, at the same abcissa value of 0.53, eq. (2) can be used to predict \(\Delta K / K_H\) values of 12.9\% and 20.2\% for the extreme \(w/h\) values.

### 4.2. Application

For purposes of applying this estimation of crack attraction to a particle, consider now a real material system such as a NiAl-Nb composite with the previously mentioned values of Young's Modulus. In NiAl, failure initiates on the grain boundaries prior to any appreciable plastic deformation, therefore an approximate value for \(d\) could be taken as roughly one-half of the grain size [16]. The value of \(d\) could similarly be approximated as a fraction of the average particle spacing which would undoubtedly be affected by the processing method as well as the actual volume fraction. The volume fraction of Nb is kept relatively low in this system, (less than 10\%) in order to retain the favorable NiAl high-temperature properties as well as the stoichiometry. Based on the low volume fraction of second phase inclusions, the average inter-particle spacing will likely be greater than the grain size. Using these approximations, it should be possible to estimate the interaction effect between the crack tip and the inclusion based on eq. (2) for various crack locations and sizes. An example of a grain size for HIPed NiAl is near 25 \(\mu m\), although the actual range of grain sizes can be very broad. The average interparticle spacing is approximately 200 \(\mu m\), and the particle aspect ratio is between 1.0-1.5 with a diameter of roughly 50 \(\mu m\) [17]. Using these approximations for \(a\) (10 \(\mu m\)) and \(d\) (75-100 \(\mu m\)) and \(A\) (2500 \(\mu m^2\)), the \([d/a](d + a)(1 / \sqrt{A})]^{1/2}\) value \(\sim 3.6-4.7\) indicates from fig. 5 that the elastic interaction between the crack and the particle is virtually zero for this configuration. For the elastic interaction to increase, the \([d/a](d + a)(1 / \sqrt{A})]^{1/2}\) parameter must decrease to a value less than one. To affect this decrease, \(A\) or \(a\) can increase, or \(d\) can decrease. Clearly the most effective way to reduce this geometrical parameter is to reduce \(d\). For exam-
ple, maintaining the $a$ and $A$ given here, $d$ must decrease to $\sim 20 \mu m$ for cracks to be attracted to particles. This leads to the idea of a zone around the particles in which crack-particle interactions are high. Applied to the NiAl material, cracks formed in such a zone would then be strongly attracted to the neighboring particle where plastic energy dissipation could stabilize deformation.

### 4.3. Generalization

In order to broaden the range of applicability of these findings past our specific case we now examine the work of other authors in an attempt to generalize trends to different combinations of elastic properties. Recall that elastic constant mismatch in two-phase materials is conveniently characterized by the Dundurs' parameters $\alpha$ and $\beta$ for plane strain as:

$$\alpha = \frac{E^+_m - E^+}{E^+_m + E^+_m} \quad \text{and} \quad \beta = \frac{\alpha}{2} \left(1 - \nu\right),$$

where $E^+ = E/(1 - \nu^2)$ is the stiffness of the matrix $(E^+_m)$ and the inclusion $(E^+_i)$ and $\nu$ is the single value of Poisson's ratio for both materials [18]. Typical two-phase engineering composites have $\alpha$ and $\beta$ values that range between $-0.6 < \alpha < 0.6$ and $\beta = \alpha/4 \pm 0.1$ [19]. A comprehensive analytical analysis of the plane strain elastic interaction between an internal crack and a circular inclusion has yielded the $\Delta K/K_H$ values plotted on the new axis format given here in fig. 6 [14]. The data show a relatively linear dependence of $\Delta K/K_H$ on $[(d/a)(a + d)(1/\sqrt{A})]\sqrt{2}$ for abscissa values on both sides of 0.9. The difference between the linear regression lines is the relative height and slope based on the magnitude and sign of $\alpha$. The second Dundurs' parameter, $\beta$, has only a very small effect on $\Delta K/K_H$ and will be considered equal to $\alpha/4$ and otherwise neglected. In an attempt to consolidate the $\Delta K/K_H$ values as a function of $\alpha$, $d$, $a$ and $A$, the data plotted in fig. 6 is replotted in fig. 7 under the ordinate format of $-\Delta K/aK_H$. This new ordinate format is chosen because the data follows an inverse proportionality to $\alpha$ and $\Delta K$ is defined as positive when $\alpha$ is negative. Figure 7 shows that good agreement exists between all of the analytical and numerical data for the range of $-0.6 < \alpha < 0.6$ and $0.3 < [(d/a)(a + d)(1/\sqrt{A})]\sqrt{2} < 1.5$. Fitting these data to lines and rewriting gives the relation

$$\frac{\Delta K}{K_H} \% \approx -\alpha[H(\alpha)x + K(\alpha)],$$

where $x = [(d/a)(a + d)(1/\sqrt{A})]\sqrt{2}$ for $x$ values $< 0.9$, and for $x > 0.9$,

$$\frac{\Delta K}{K_H} \% \approx \beta[I(\alpha)],$$

where

\begin{align*}
H(\alpha) &= 30.6\alpha^2 + 21.1\alpha - 87.4, \\
K(\alpha) &= -10.4\alpha^2 - 21.4\alpha + 80.5, \\
I(\alpha) &= 11.4\alpha^2 - 3.6\alpha + 7.3.
\end{align*}
Equations (5–9) provide a very simple method for estimating the interaction effects between a circular particle and an internal, radial plane-strain crack in terms of the geometry of the specimen and its relative elastic constants. Mueller and Schmauder's analytical results for the internal crack are fully consistent with the numerical elastic calculations given above for a side-cracked panel for various inclusion shapes and aspect ratios [14]. Turning attention once again to eq. (2) and recalling that \( \alpha = -0.35 \) in the side-cracked specimen plots shown above, it is possible to conclude that in the most general sense we may express the relation between the crack tip and particle as a function of both the aspect ratio and elastic mismatch by

\[
\frac{\Delta K}{K_H} \% \approx \frac{-\alpha}{0.35} \left[ U \left( \frac{w}{h} \right) x + V \left( \frac{w}{h} \right) \right]
\]

which is equivalent to

\[
\frac{\Delta K}{K_H} \% \approx -\alpha \left[ U' \left( \frac{w}{h} \right) x + V' \left( \frac{w}{h} \right) \right],
\]

where

\[
U' = 11.4 \left( \frac{w}{h} \right) - 106.6, \quad \text{and} \quad V' = -13.3 \left( \frac{w}{h} \right) + 116.3
\]

for \( x < 1 \) and \( 0.3 \leq w/h \leq 3 \), where \( x = \left[ \frac{(d/a)(d + a)}{\sqrt{A}} \right]^{1/2} \). For values of \( x > 1 \), the simple expression

\[
\frac{\Delta K}{K_H} \% \approx -10\alpha
\]

provides a good approximation for all reasonable \( \alpha \) and \( w/h \). It has thus been shown that for any combination of elastic constants and reasonable \( w/h \), Equations (11) and (14) may be used as good estimates of \( \Delta K/K_H \) for particles located in the crack-plane.

5. Summary and conclusions

The model results detailed above provide a clear and concise method for evaluating the attraction or repulsion between a crack and a particle in an elastic composite based on the geometric and elastic parameters of the specimen. Specifically, for particles to influence crack growth \( (\alpha < 0) \) or arrest \( (\alpha > 0) \) the parameter \( x = \left[ \frac{(d/a)(d + a)}{\sqrt{A}} \right]^{1/2} \) must satisfy the condition \( x \leq 1 \) for any combination of material constants. In terms of geometrical components this implies that a zone around the particles exists in the particle mid-plane up to a distance of

\[
d \sim \frac{-a}{2} \left[ 1 - \left( 1 + \frac{4\sqrt{A}}{a} \right) \right]
\]

for a given particle size \( (A) \) and a crack length \( (a) \) in which elastic crack-particle interactions are significant. For cracks that approach particles above or below the particle mid-plane, this zone radius is a more complicated function [20]. The extent and nature of this in-plane interaction can easily be approximated by eqs. (11) and (14) for any combination of \( d, a, w/h, \alpha, \beta \) and \( A \). Of these variables, the largest influence on \( \Delta K/K_H \) for a given material system is the crack-particle separation, \( d \). The particle shape \( (w/h) \) has a smaller influence on the magnitude of \( \Delta K/K_H \) with the effects of \( A \) and \( a \) being smaller still. If some flexibility is allowed in the material combination, \( \alpha \) can also bear a very strong influence on crack-tip stress intensity factors.

Applied to actual material development, the results above indicate that a close particle spacing would be most effective for covering the majority of the specimen with zone regions. Given a range of possible volume fractions, grain sizes and other as-processed variables, the above results may be used to estimate the effectiveness of the particles at attracting cracks. The future calculations related to this work will involve particle plasticity and multi-particle systems in order to serve as a still more accurate guide in the development and understanding of deformation and failure in general material combinations.

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References

[17] Personal communication, Dr. A. Wanner, MPI.