Analysis of Whisker-Toughened Ceramic Components—A Design Engineer’s Viewpoint

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Page 7: The distributions of risk of rupture intensity depicted in figures 4 and 6 should be interchanged.
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Summary

The use of ceramics components in gas turbines, cutting tools, and heat exchangers has been limited by the relatively low flaw tolerance of monolithic ceramics. The development of whisker-toughened ceramic composites offers the potential for considerable improvement in fracture toughness as well as strength. However, the variability of strength is still too high for the application of deterministic design approaches. This report reviews several phenomenological reliability theories proposed for this material system, and reports on the development of a public domain computer algorithm. This algorithm, when coupled with a general-purpose finite element program, predicts the fast fracture reliability of a structural component under multiaxial loading conditions.

Introduction

The potential advantages of ceramic matrix composites include increased fracture toughness, and creep and corrosion resistance at very high service temperatures. The primary applications under consideration are advanced turbine engine components, cutting tool bits, heat exchangers, and aerospace components (specifically those of the National Aerospace Plane). Considering that these composites will be produced from nonstrategic materials, it is not surprising that concerted research efforts are under way both in the field of materials science (to advance processing techniques) and in the field of engineering mechanics (to develop design methodologies for these material systems).

The material system of interest in this report is the whisker-toughened ceramic matrix composite. Analysis of components fabricated from this material requires a departure from the design philosophy (i.e., the factor of safety approach) prevalent in designing metallic structural components, which are more tolerant of flaws. Since failure of components fabricated from this material is governed by the scatter in strength, statistical design approaches must be used. The primary objective of this report is to review several phenomenological failure models and to report on the development of a public domain computer algorithm which, when coupled with a general-purpose finite element program, predicts the fast fracture reliability of a structural component under multiaxial loading conditions. The present version of this algorithm has been given the acronym TCARES (Toughened Ceramics Analysis and Reliability

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Evaluation of Structures) and is a direct offspring of the CARES (a.k.a. SCARE) program (ref. 1), which has found widespread use in the design of monolithic ceramic components.

In addition to capturing the inherent scatter in strength, the reliability analysis of components fabricated from whisker-toughened ceramics must account for material symmetry imposed by whisker orientation. A noninteractive macroscopic model has been presented that accounts for the transversely isotropic material symmetry (S.F. Duffy and S.M. Arnold, Noninteractive Macroscopic Statistical Failure Theory for Whisker Reinforced Ceramic Composites, to be published in J. Compos. Mater.) often encountered in hot-pressed and injection-molded whisker-toughened ceramics. A similar model (ref. 2) has been proposed for whisker-toughened ceramics with orthotropic material symmetry. This continuum approach excludes any consideration of the microstructural events that involve interactions between individual whiskers and the matrix. Other authors have addressed fracture of ceramic matrix composites on a more local scale. A model based on probabilistic principles has been developed to compute an increased energy absorption during fracture due to whisker pull-out (ref. 3). The processes of crack deflection (ref. 4) and crack pinning (ref. 5) have also been addressed. The latter two approaches are founded in deterministic fracture mechanics. Since these crack mitigation processes strongly interact, it is difficult to experimentally detect or analytically predict the sequence of mechanisms leading to failure.

A more feasible approach is to compute reliability in terms of macrovariables by using a continuum-based criterion. This underscores a fundamental difference that exists between the materials scientist and the engineer. The materials scientist focuses on mechanisms of failure at the microstructural level, and the engineer focuses on this issue at the component level. The failure models currently incorporated into the computer algorithm TCARES adopt the engineer’s viewpoint. This point of view implies that the material element under consideration is small enough to be homogeneous in stress and temperature, yet large enough to contain a sufficient number of whiskers such that the element is a statistically homogeneous continuum. This does not imply that the microscopic and macroscopic levels of focus are mutually exclusive. Indeed, a close relationship must exist between the materials scientist and the design engineer so as to develop better failure models to facilitate the use of ceramic materials in structural components.

**Noninteractive Reliability Models**

Here, a continuum is considered to be a chain composed of links connected in series. Therefore, the overall strength of the continuum is governed by the strength of its weakest link. It is further assumed that the events leading to failure of an individual link are not influenced by any other link in the chain. Defining \( f \) as the probability of failure of an individual link gives

\[
f = \psi \Delta V
\]

where \( \Delta V \) denotes an increment in volume and \( \psi \) is a failure function per unit volume of material. By taking \( r \) as the reliability of an individual link, then

\[
r = 1 - \psi \Delta V
\]

If the failure of an individual link is considered a statistical event, and if these events are assumed to be independent, then the reliability of the continuum, denoted as \( R \), is given as

\[
R = \lim_{N \to \infty} \left\{ \prod_{i=1}^{N} \left[ 1 - \psi(x_i) \Delta V \right] \right\}
\]

where \( N \) denotes the number of links and \( \psi(x_i) \) is the failure function per unit volume at position \( x_i \) within the continuum. Lowercase Roman letter subscripts here and in the following expressions denote tensor indices with an implied range from 1 to 3. Greek letter subscripts and uppercase italic letters are associated with products or summations with ranges that are explicit in each expression. Alternatively, the reliability of the continuum is given by the following expression

\[
R = \exp \left( - \int \psi \, dV \right)
\]

where the integral within the bracket is referred to as the risk of rupture.

Depending on fabrication, a whisker-toughened composite may have isotropic, transversely isotropic, or orthotropic material symmetry. The principle of independent action (PIA) would be an appropriate first approximation macroscopic theory for isotropic whisker composites. In this instance the failure function \( \psi \) would depend only on stress or the principal invariants of stress; that is,

\[
\psi = \psi(\sigma_{ij}) = \psi(\sigma_1, \sigma_2, \sigma_3)
\]

where \( \sigma_{ij} \) is the Cauchy stress tensor and \( \sigma_1, \sigma_2, \) and \( \sigma_3 \) are the associated principal stresses.

However, for transversely isotropic whisker composites, the failure function must also reflect material symmetry. This requires that

\[
\psi = \psi(\sigma_{ij}, a_i)
\]

where \( a_i \) is a unit vector that identifies a local material orientation. This orientation, depicted in figure 1, is defined as the normal to the plane of isotropy. The sense of \( a_i \) is...
immaterial, and thus its influence is taken through the product \( a_1a_j \); that is,

\[
\psi = \psi(a_{ij}, a_i, a_j)
\]  \hspace{1cm} (7)

Note that \( a_1a_j \) is a symmetric second-order tensor, the trace of which satisfies the identity \( a_1a_1 = 1 \). Furthermore, the stress and local preferred direction may vary from point to point in the continuum. Thus equation (7) implies that the stress field and the unit vector field (i.e., \( \sigma_j(x_k) \) and \( a_j(x_k) \)) must be specified to define \( \psi \).

For orthotropic composites the failure function must also reflect the appropriate material symmetry. This requires that

\[
\psi = \psi(a_{ij}, a_1a_1, b_i b_j)
\]  \hspace{1cm} (8)

where \( a_i \) (a different vector than the one used for transverse isotropy) and \( b_i \) are unit vectors that identify local material orientations. These vectors are assumed to be orthogonal such that \( a_1b_i = 0 \).

Since \( \psi \) is a scalar valued function dependent on second-order tensors, the form of \( \psi \) must remain invariant under proper orthogonal transformations. This requires the function to be insensitive to the global coordinate system used to define the stress tensor and material directions. Through the use of invariant theory, a finite set of invariants known as an integrity basis can be developed for the isotropic, transversely isotropic, and orthotropic material symmetries (table I). The individual invariants of each integrity basis can be likened to a basis vector that helps to span a particular vector space (e.g., the set of unit vectors that span the Cartesian space). A slightly different set of invariants that correspond to physical mechanisms related to failure is constructed from each integrity basis. (See table II for a brief description of each invariant and fig. 2 for a graphical interpretation.) These invariants can be identified with a principal stress or a component of the stress tractions coincident with a material direction.

The invariants used to form \( \psi \) are assumed to act independently in producing failure such that \( \psi \) has the following general form:

\[
\psi = \left( \frac{I_1}{\beta_1} \right)^{\alpha_1} + \ldots + \left( \frac{I_N}{\beta_M} \right)^{\alpha_M}
\]  \hspace{1cm} (9)

where \( N = 3 \) and \( M = 1 \) for isotropy, \( N = 4 \) and \( M = 3 \) for transverse isotropy, and \( N = M = 5 \) for orthotropy (table III). In association with each invariant, the \( \alpha \)'s correspond to Weibull shape parameters and the \( \beta \)'s correspond to Weibull scale parameters. A variety of test methods could be used to determine these parameters. One approach is to obtain the data associated with the normal stress tractions from fast fracture of simple bend test specimens, often referred to as modulus of rupture (MOR) bars. The Weibull parameters associated with shear tractions would be obtained from appropriate shear strength tests. It is further assumed that compressive principal stresses and compressive stresses associated with a material orientation do not contribute to failure.

**TCARES Algorithm**

The basic data requirements of TCARES (fig. 3) closely follow the structure of its parent code CARES. The algorithm requires the stress analysis from a general-purpose finite
TABLE II.—INVARlANTS ASSOCIATED WITH PHYSICAL MECHANISMS
DIRECTLY RELATED TO FAILURE

<table>
<thead>
<tr>
<th>Material symmetry</th>
<th>Invariants used in ( \psi ) function</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropy</td>
<td>( \bar{l}_1 = 0 )</td>
<td>Principal stresses; functionally dependent on the first three invariants of stress</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_1 = 0 )</td>
<td>Normal stress component of stress traction associated with ( a_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_1 = 0 )</td>
<td>Shear stress component of stress traction associated with ( a_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_1 = 0 )</td>
<td>Maximum normal stress in plane of isotropy</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_1 = 0 )</td>
<td>Minimum normal stress in plane of isotropy</td>
</tr>
<tr>
<td>Transverse isotropy</td>
<td>( \bar{l}_1 = I_4 )</td>
<td>Normal stress component of stress traction associated with ( a_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_2 = [I_5 - (I_4)^2]^{1/2} )</td>
<td>Shear stress component of stress traction associated with ( a_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_3 = \frac{1}{2}(I_1 - I_4) + R )</td>
<td>Normal stress component of stress traction associated with ( b_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_4 = \frac{1}{2}(I_1 - I_4) - R )</td>
<td>Shear stress component of stress traction associated with ( b_l )</td>
</tr>
<tr>
<td>Orthotropy</td>
<td>( \bar{l}_1 = I_4 )</td>
<td>Normal stress component of stress traction associated with ( a_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_2 = [I_5 - (I_4)^2]^{1/2} )</td>
<td>Shear stress component of stress traction associated with ( a_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_3 = I_6 )</td>
<td>Normal stress component of stress traction associated with ( b_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_4 = [I_5 - (I_4)^2]^{1/2} )</td>
<td>Shear stress component of stress traction associated with ( b_l )</td>
</tr>
<tr>
<td></td>
<td>( \bar{l}_5 = I_1 - I_4 - I_6 )</td>
<td>Normal stress in direction defined by cross product of ( a_l ) and ( b_l )</td>
</tr>
</tbody>
</table>

\[ R = \left( \frac{1}{2}I_1 \right)^2 - I_5 + \left( \frac{1}{4}I_4 \right)^2 - \left( \frac{1}{4}I_4 \right)^2 + \left( \frac{1}{8}I_4^2 \right) \]

(a) Transverse isotropy.
(b) Orthotropy.

Figure 2.—Invariants associated with transverse isotropy and orthotropy.

WARES requires certain information from the finite element code. Currently, the preliminary version of TCARES is compatible with MSC/NASTRAN, although it is anticipated that future versions compatible with the MARC, ADINA, and ANSYS finite element codes will be available. The algorithm allows the user to specify temperature-dependent statistical material parameters for each material symmetry. Alternatively, the program has the capability to estimate statistical parameters from fracture data obtained from uniaxial tensile or flexural specimens. (Details of this capability can be found in ref. 6.) The preceding section on noninteractive theoretical models implies a volume flaw analytical approach. It is quite possible that the surface and volume of a structural component will fail because of distinctly different flaw populations. Accordingly the TCARES program has the capability to separately conduct surface and volume reliability analyses. The program produces as bulk output a summary of input from the finite element code, element statistical properties, element survival probabilities, and an overall component survival probability.

TCARES requires certain information from the finite element structural analysis. This includes element volumes, nodal temperatures, centroidal or nodal stresses, element principal stresses (for PIA analysis), and element identification numbers. The current version of TCARES assumes that the nodal stresses from the finite element code are provided relative to the local material orientation for transversely isotropic and orthotropic materials. This precludes having to input material orientation vectors for each finite element.

The TCARES user input requirements are grouped into three categories. (See table IV.) The first category, entitled master control input, defines control indices for stress and graphics output, the number of component materials, and information regarding the finite element code and mesh. The second
TABLE III.—FUNCTIONAL FORMS OF $\psi$
CORRESPONDING TO MATERIAL SYMMETRY

<table>
<thead>
<tr>
<th>Material symmetry</th>
<th>Functional form of $\psi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropy $N = 3$, $M = 1$</td>
<td>$\psi = \left(\frac{a_1}{b_1}\right)^{a_1} + \left(\frac{a_2}{b_2}\right)^{a_2} + \left(\frac{a_3}{b_3}\right)^{a_3}$</td>
</tr>
<tr>
<td>Transverse isotropy $N = 4$, $M = 3$</td>
<td>$\psi = \left(\frac{a_1}{b_1}\right)^{a_1} + \left(\frac{a_2}{b_2}\right)^{a_2} + \left(\frac{a_3}{b_3}\right)^{a_3} + \left(\frac{a_4}{b_4}\right)^{a_4} + \left(\frac{a_5}{b_5}\right)^{a_5}$</td>
</tr>
<tr>
<td>Orthotropy $N = M = 5$</td>
<td>$\psi = \left(\frac{a_1}{b_1}\right)^{a_1} + \left(\frac{a_2}{b_2}\right)^{a_2} + \left(\frac{a_3}{b_3}\right)^{a_3} + \left(\frac{a_4}{b_4}\right)^{a_4} + \left(\frac{a_5}{b_5}\right)^{a_5}$</td>
</tr>
</tbody>
</table>

From Simple to Complex Geometries

Multiaxial experiments are a necessity to assess the accuracy of the noninteractive modeling approach. One experimental avenue highlighted here is the application of thermomechanical loads to tubular specimens. Initially, a thick-walled tube subjected to an applied torque is considered. A second problem is presented where the same thick-walled tube is subjected to a simultaneous application of internal pressure and axial torque. In all applications considered, isothermal conditions are assumed. However, the algorithm is capable of non-isothermal analyses if the user specifies the values of the Weibull parameters at a sufficient (and appropriate) number of temperature values. Unfortunately, at the present time no data base exists to properly characterize the multiaxial
statistical parameters for a whisker-toughened ceramic, although efforts (ref. 7) are under way to accomplish this goal. Thus, an assessment of the program output relative to actual structural component data is reserved for a later date. For the examples that follow, Weibull statistical parameters are assumed for the purpose of illustration; however, the values adopted are well within the range of the sparse data that can be found in the open literature (refs. 8 to 10).

To test the validity of the reliability calculations performed by the program, a comparison of output with a hand calculation is presented for the aforementioned simple structural problem, that is, a thick-walled tube subjected to an axial moment or torque. It is assumed that the cylinder is fabricated from a whisker-toughened ceramic material having an orthotropic material symmetry such that $a_1 = (0,0,1)$ and $b_1 = (0,1,0)$ at every point in the structure. A cylindrical coordinate system readily lends itself to this application; hence, $a_1$ is directed along the $z$-axis of the cylinder and $b_1$ is oriented in the $\theta$ (circumferential) direction. With this geometry, material symmetry, and load condition, only the two terms (see table III) in the failure function associated with shear tractions are nonzero, and $\psi$ takes the form

$$\psi = \left( \frac{Tr}{J\delta_2} \right)^{\alpha_2} + \left( \frac{Tr}{J\delta_4} \right)^{\alpha_4} \tag{10}$$

where $T$ is the applied torque, $r$ is the radius, and $J$ is the polar moment of inertia. Assuming an inner radius of 1 cm, an outer radius of 5 cm, and a length of 5 cm gives

$$R = \exp \left( - \iiint \psi r \, dr \, d\theta \, dz \right)$$

$$= \exp \left( -10\pi \int \psi r \, dr \right) \tag{11}$$
For dimensionless reliability, the Weibull scale parameters \((\beta_1, \ldots, \beta_5)\) have units of stress \(\times\) (volume)\(^{1/6}\), and the Weibull shape parameters are unitless. With \(\alpha_2 = 10\), \(\beta_2 = 15000\), \(\alpha_4 = 6.5\), \(\beta_4 = 10000\) (the other Weibull parameters can be stipulated arbitrarily), and \(T = 7500\) N m, the above integration yields an overall reliability of 83.6 percent. The problem was also modeled by using MSC/NASTRAN to generate a numerical solution for the stress distribution. The model was composed of 1500 eight-node elements (the stresses were within 2 percent of the closed form solution) which generated an overall component reliability of 81.8 percent. Figure 4 is a color plot of the variation of \(\psi\) in a quarter section of the component. Note that \(\psi\) (risk of rupture intensity) is a measure of reliability independent of the element geometry, and that it attains a maximum value along the outer edge of the tube.

Next, consider the same tube, subject to the conditions stated in the preceding paragraph, with an additional applied internal pressure of 70 MPa. Here \(\alpha_3\) and \(\beta_3\) cannot be stipulated arbitrarily and take values of \(\alpha_3 = 7.5\) and \(\beta_3 = 12000\). The overall component reliability decreases to 77.4 percent. For this load case the circumferential stress is a maximum at the inner radius, and it decreases nonlinearly through the thickness. The shear stress from the applied torque is a minimum at the inner radius, and it increases linearly with the radius. Given this multiaxial stress distribution, one expects the maximum risk of rupture intensity to occur at some point midway through the thickness. However, this is not the case, as is evident in figure 5. The maximum risk of rupture intensity occurs at the inner radius, and much of the inner volume of the tube remains relatively "cold." This underscores the need of not only considering overall component reliability, but also giving consideration as to where local "hot" spots occur within.
a component. If this particular component were to fail, one would expect the failure to originate in the vicinity of the inner radius.

Overall component reliability can be adversely affected by either increasing the stress distribution in additional regions of the component (the so-called size effect), or by dramatically increasing the stress locally (thereby increasing the chance of failing a single link in the chain). Increasing the internal pressure of the previous example to 100 MPa sharply decreases the component reliability to 36 percent. Figure 6 depicts the variation of $\psi$ throughout the component. It appears that the additional affected region of the component is minimal. However, $\psi$ changes two orders of magnitude along the inner radius. Although not depicted here, the overall component reliability of the tube subjected to only an internal pressure of 100 Mpa is 44 percent, indicating that the major source in the degradation of reliability is the internal pressure.

Concluding Remarks

The applications presented here represent very straightforward structural analyses. Similar calculations and graphical interpretations can be carried over into designs with much more complex geometry and boundary conditions.

Recent advances in processing whisker-toughened ceramics have resulted in the reduction of inhomogeneities, uniform whisker distributions, and increasingly dense matrices, all of which have greatly improved the reliability of this material system. However, the variability of strength is still too high for the application of deterministic design approaches. Statistical design methodologies must be used not only to account for the scatter in ultimate strength, but also to account for decreasing bulk strength with increasing component volume (the so-called size effect). If the orientation of the whiskers is such that an anisotropic material symmetry is imparted, this must also be accounted for. Several phenomenological failure theories that take into consideration these issues in a macroscopic sense have been reviewed. In addition, a computer algorithm has been discussed that incorporates these theories and that is capable of predicting reliability given the state of stress and temperature distribution within a component.

References

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**Abstract**

The use of ceramics components in gas turbines, cutting tools, and heat exchangers has been limited by the relatively low flaw tolerance of monolithic ceramics. The development of whisker-toughened ceramic composites offers the potential for considerable improvement in fracture toughness as well as strength. However, the variability of strength is still too high for the application of deterministic design approaches. This report reviews several phenomenological reliability theories proposed for this material system, and reports on the development of a public domain computer algorithm. This algorithm, when coupled with a general-purpose finite element program, predicts the fast fracture reliability of a structural component under multiaxial loading conditions.