MICROSTRUCTURAL THERMAL STRESSES IN CERAMIC MATERIALS

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(Received 1 May 1987; in revised form 28 September 1987)

Abstract

The problem addressed concerns the analytical characterization of the state of residual stress in a polycrystalline ceramic material following cooling from the fabrication temperature. It is shown that, under mild assumptions on the behavior and microstructure of the material, the covariance matrix of the microstructural residual stresses can be obtained in closed form from the equations of elasticity. The analysis does not take thermally induced microcracking into consideration and the solid is idealized as remaining essentially intact during the cooling process. However, the results so obtained are subsequently used to derive first-order estimates of microcrack densities.

1. Introduction

Residual stresses typically arise in ceramic materials due to mismatches between the thermal expansion coefficients of adjacent grains (BOAS and HONEYCOMBE, 1944; LIKHACHEV, 1961; BUSSSEM et al., 1966; BUSSSEM and LANGE, 1966). As the material is cooled from the fabrication temperature, the anisotropy and random orientation of the grains result in incompatible thermal strains which in turn give rise to self-equilibrated microstructural stresses. In some cases, the magnitude of these stresses is large enough to produce considerable microcracking along grain boundaries. For instance, PbTiO$_3$ completely crumbles below its phase transformation temperature when the grain size is larger than a critical value (RIE and POHANKA, 1979). In general, the extent of microfracturing exhibits great sensitivity to the grain size, being more severe in coarse grained ceramics. Spontaneous microcracking may have a significant influence on the mechanical, optical and thermal properties of the material. It is therefore a matter of practical interest to develop an understanding which can eventually lead to methods for controlling or preventing such cracking.

The generation of thermally induced residual stresses in polycrystalline ceramics has been the focus of several studies. BOAS and HONEYCOMBE (1944) derived a rough estimate of the magnitude of the residual stresses. LIKHACHEV (1961) idealized the problem as that of an anisotropic grain embedded in a rigid matrix endowed with the average thermal expansion coefficients of the polycrystalline body. LIKHACHEV's analysis was subsequently...
refined by BUESSEM and LANGE (1966). More recently, EVANS (1978) (see also Fu and EVANS, 1985) carried out an analysis based on ESHELBY's method. Their approach is deterministic and relies on simplified two-dimensional models.

In this paper, we endeavor to obtain an analytical characterization of the statistical properties of the residual stress field directly from the equations of linear elasticity. To make the analysis tractable, a number of simplifying assumptions are made. Firstly, we neglect the microstructural anisotropy and heterogeneity of the elastic moduli. Thus, the solid is idealized as being elastically homogeneous and isotropic but thermally heterogeneous. It is shown in Appendix 3 that, for small deviations from homogeneity, the influence of elastic heterogeneity is indeed a second-order effect and can be neglected to a first approximation. Interestingly, although the overall effect of elastic anisotropy can be expected to be small compared to that of thermal anisotropy, the former may induce local stress fluctuations of considerable importance. For instance, TVERGAARD and HUTCHINSON (1987) have shown that elastic anisotropy results in stress concentrations at grain junctions which may promote microcracking.

As a further simplifying assumption, the effect of microcracking is neglected and the body is idealized as remaining essentially intact. This limits the validity of the analysis to cases in which the extent of microcracking is small. However, we show that for many systems of practical interest this limitation is not particularly stringent. A further assumption is that the cooling process is slow enough that the temperature field can be taken to be uniform over the body. Finally, the grains are assumed to be uniform in size and have random orientations.

Within this idealized framework, we show that the covariance matrix of the residual stresses can be computed analytically in closed form. If one further assumes that the residual stresses at a point are normally distributed, the computed covariance matrix provides a complete characterization of the statistical distribution of residual stresses. For Al₂O₃, the computations are seen to be in good agreement with the available observational evidence. The analytical results are then employed to derive first-order estimates of the microcrack densities. In this application, we assume that microcrack nucleation at grain boundary facets is governed by a critical normal stress.

### 2. FIELD EQUATIONS

We start by formulating the field equations governing the microscopic response of a polycrystalline ceramic material undergoing cooling. The primary focus of the analysis is the characterization of the spatial distribution of residual stresses. To make the analysis tractable, several simplifying assumptions are made. Firstly, the coupling between thermal stresses and microcracking is not taken into account and the material is idealized throughout as being flawless. However, the results so obtained are subsequently utilized to derive first-order estimate of microcrack densities. We further assume that the material behaves linear elastically, so that the stress–strain relations can be expressed

\[ \sigma_{ij}(x) = D_{ijkl}(x)\varepsilon_{kl}(x) - \beta_{ij}(x)\theta(x), \]

where \( \sigma(x) \), \( \varepsilon(x) \) and \( \theta(x) \) signify the stress, strain and temperature fields, \( D(x) \) the elastic moduli, and one write \( \alpha(x) \).

Both the elastic and the thermal fluctuations are random. In particular, the random field \( \varepsilon(x) \) is assumed to have Gaussian probability density functions, and the field \( \theta(x) \) is assumed to have exponential probability density functions. Thus, the stress–strain relations can be expressed as

\[ \sigma_{ij}(x) = D_{ijkl}(x)\varepsilon_{kl}(x) - \beta_{ij}(x)\theta(x), \]

where \( \sigma(x) \), \( \varepsilon(x) \) and \( \theta(x) \) signify the stress, strain and temperature fields, \( D(x) \) the elastic moduli, and one write \( \alpha(x) \).

By linearity, the

\[ u_i(x) = \]
moduli, and one writes \( \beta_{ij}(\mathbf{x}) = D_{ijkl}(\mathbf{x})\alpha_{kl}(\mathbf{x}) \) in terms of the thermal expansion coefficients \( \alpha(\mathbf{x}) \).

Both the elastic moduli and the thermal expansion coefficients exhibit microstructural fluctuations which reflect the heterogeneities of the polycrystalline ensemble. In particular, since \( \beta \) is anisotropic and the grains are randomly oriented, a mismatch exists between the thermal properties of adjacent grains. Thus, whereas the principal values \( \beta_{kk}, \alpha = 1, 2, 3 \) of \( \beta \) can be regarded as uniform material constants, its principal directions vary randomly from grain to grain. Similar structure can be expected of the elastic moduli. However, to simplify the analysis we treat \( D \) as being homogeneous and isotropic. Thus, we idealize the body as being elastically homogeneous but thermally heterogeneous. This idealization is justified in Appendix 3 on the basis of a perturbation expansion. Indeed, it is shown that, for small deviations from homogeneity, the effect of elastic anisotropy is of second order and can be neglected to a first approximation.

In addition, we assume that the process of cooling is slow enough that the temperature \( \theta \) can be considered to be uniform over the body. Under these conditions, combination of Eq. (2.1) with the equations of equilibrium and compatibility yields Navier’s equation

\[
\mu u_{i,k} + (\lambda + \mu) u_{k,ki} - \beta_{k,k} \theta = 0
\]  

(2.2)

with thermally induced body forces. Here \( u(\mathbf{x}) \) is the displacement field and \( \lambda \) and \( \mu \) are the Lame constants.

Since the primary objective of the analysis is the characterization of microscopic fields, a local macroscopic neighborhood of the body will be idealized as being unbounded in all directions. Furthermore, macroscopic variables can be identified with the spatial averages of the micromechanical fields. Thus, for instance, the macroscopic or average stress is given by

\[
\langle \sigma_{ij} \rangle = \lim_{V \to \infty} \frac{1}{V} \int_{V} \sigma_{ij} \, dV,
\]  

(2.3)

where here and subsequently the angle brackets are used to denote spatial averaging as indicated. The value of a field in excess of its average will be referred to as its fluctuation component and denoted by means of a prefix \( \delta \). Thus, for instance, the fluctuation or residual stress field is given by

\[
\delta \sigma_{ij}(\mathbf{x}) = \sigma_{ij}(\mathbf{x}) - \langle \sigma_{ij} \rangle.
\]  

(2.4)

By linearity, the general solution of (2.2) can be expressed in integral form as

\[
u_k(\mathbf{x}) = U_k(\mathbf{x}) - \theta \int g_{ij}(\mathbf{x} - \mathbf{x}') \delta \beta_{j,k}(\mathbf{x}') \, dV' = U_k(\mathbf{x}) - \theta g_{ij} * \delta \beta_{j,k},
\]  

(2.5)

where the symbol \( * \) is used to denote the convolution operator and use has been made of the identity \( \beta_{ij} = \langle \beta_{ij} \rangle + \delta \beta_{ij} \). The Green’s function \( g(\mathbf{x}) \) is a solution of the problem

\[
D_{ijkl} g_{km,ij}(\mathbf{x}) + \delta_{lm} \delta(\mathbf{x}) = 0,
\]  

(2.6)

where \( \delta(\mathbf{x}) \) signifies Dirac’s delta. The term \( U_k(\mathbf{x}) \) in (2.5) represents an arbitrary
solution of the homogeneous Navier equations and can be regarded as the macroscopic displacement field. From (2.5) the strains are computed to be

\[ \varepsilon_{ij} = \langle \varepsilon_{ij} \rangle - \theta \frac{1}{2} (g_{i,j} + g_{j,i}) \delta \beta_{R,k}, \]  

(2.7)

where

\[ \langle \varepsilon_{ij} \rangle = \frac{1}{2} (U_{i,j} + U_{j,i}) \]  

(2.8)

is the average or macroscopic strain. Equation (2.7) can be recast as

\[ \delta \varepsilon_{ij} = -\theta \frac{1}{2} (g_{i,j} + g_{j,i}) \delta \beta_{R,k}, \]  

(2.9)

in view of the definition \( \delta \varepsilon_{ij} = \varepsilon_{ij} - \langle \varepsilon_{ij} \rangle \) of the fluctuation strains. Inserting (2.9) into (2.1) we finally obtain

\[ \delta \sigma_{ij} = -D_{ijml} \theta \frac{1}{2} (g_{ml,n} + g_{nl,m}) \delta \beta_{R,k} - \theta \delta \beta_{ij}, \]  

(2.10)

which relates the fluctuation or residual stress field to the microscopic fluctuations in the thermal expansion coefficients.

In view of the linearity of the problem and the fact that the domain of analysis coincides with all of \( \mathbb{R}^3 \), the use of Fourier transform methods suggests itself as a natural possibility. Several key properties of Fourier transforms are assembled in Appendix I for later reference. A simple calculation shows that the Fourier transform of Green's function \( g \) takes the form

\[ \hat{g}_{ij}(k) = \frac{1}{\mu k^2} \left[ \delta_{ij} - \frac{\lambda + \mu}{\lambda + 2\mu} \xi_i \xi_j \right], \]  

(2.11)

where \( k \) is the wave number vector, \( k = |k| \), \( \xi = k/k \) and a superimposed hat is henceforth used to denote the Fourier transform of a function. Taking the Fourier transform of (2.10) yields

\[ \delta \hat{\sigma}_{ij} = D_{ijmn} \hat{\theta} \hat{g}_{km} \delta \hat{\beta}_{R,k} - \theta \delta \hat{\beta}_{ij}. \]  

(2.12)

Finally, inserting (2.11) into (2.12) we obtain a relation

\[ \delta \hat{\sigma}_{ij} = \theta A_{ijkl} \delta \hat{\beta}_{kl}, \]  

(2.13)

where

\[ A_{ijkl} = \frac{\lambda}{\lambda + 2\mu} \delta_{ij} \xi_k \xi_l + \frac{1}{2} (\delta_{ik} \xi_j \xi_l + \delta_{il} \xi_j \xi_k) + \frac{2(\lambda + \mu)}{\lambda + 2\mu} \xi_i \xi_j \xi_k \xi_l - \delta_{ik} \delta_{jl}. \]  

(2.14)

Equation (2.13) places the fluctuations in the thermal expansion coefficients in correspondence with the residual stress field, and constitutes the basic building block for the calculations that we have seen that the influence of the residual stress and not on its Young temperature \( \theta \) enters the determination of the covariance matrix of the residual stresses. This linearity, however, becomes significant.

3.

Whereas formally it is of limited value to require knowledge of the microstructure of the materials, it is of considerable practical interest to determine the covariance matrix of the fluctuations. Furt further refinement Gaussian, the covariances distribution. Our point of departure is the fact that the covariance matrix is not defined readily. Furt further refinement Gaussian, the covariance matrix is not defined readily.

The precise meaning Substituting (2.13) into (2.12) yields

\[ \delta \hat{\sigma}_{ij} = \theta A_{ijkl} \delta \hat{\beta}_{kl}. \]  

Next we turn our attention to the introduction of the autocovariance function

\[ \text{autocovariance function} \]

But, by virtue of the Fourier transform, evaluating the sought correlation function...
for the calculations that follow. Some features of (2.13) are noteworthy. Firstly, it is
seen that the influence tensor $A$ depends only on the Poisson ratio $v$ of the material,
and not on its Young’s modulus. Furthermore, it is interesting to note that the average
temperature $\theta$ enters (2.13) linearly. Thus, for a given microstructure, the magnitude
of the residual stresses is predicted to be proportional to the temperature excursion.
This linearity, however, is likely to be lost as soon as the effect of microcracking
becomes significant.

3. COVARIANCE MATRIX OF THERMAL STRESSES

Whereas formally Eq. (2.13) determines the sought residual stress field, in practice
it is of limited value as it stands since it requires an exact pointwise description of the
microstructure of the solid. Indeed, as noted by [Beran 1965], rarely does one have
microstructural information beyond two-point correlations. Thus, solutions which
require knowledge of higher order correlations are likely to be impractical. Guided
by these observations, we narrow the scope of subsequent calculations to the deter-
imination of the covariance matrix of the fluctuation stresses. As we shall see, such
covariance matrix only involves the two-point correlations of $\delta \beta$, which can be deter-
mined readily. Furthermore, if the fluctuation stresses at a point are assumed to be
Gaussian, the covariance matrix provides a complete description of their statistical
distribution.

Our point of departure is Eq. (A1.2a) from Appendix 1, which allows one to express
the covariance matrix of $\delta \sigma$ as

$$\langle \delta \sigma_{ij} \delta \sigma_{kl} \rangle = \lim_{\nu \rightarrow \infty} \frac{1}{V} \int \delta \sigma^*_\nu(k) \delta \sigma_{kl}(k) \, d^3k. \quad (3.1)$$

The precise meaning of the limiting process taken in (3.1) is discussed in Appendix 1.
Substituting (2.13) into (3.1) we obtain

$$\langle \delta \sigma_{ij} \delta \sigma_{kl} \rangle = \theta^2 \lim_{\nu \rightarrow \infty} \frac{1}{V} \int A^*_\nu A A^* \delta \beta^*_\nu(\mathbf{k}) \delta \beta_{kl}(\mathbf{k}) \, d^3k. \quad (3.2)$$

Next we turn our attention to the computation of the power spectrum

$$P_{ijkl}(k) = \lim_{\nu \rightarrow \infty} \frac{1}{V} \delta \beta^*_\nu(\mathbf{k}) \delta \beta_{kl}(\mathbf{k}). \quad (3.3)$$

which is the element of (3.2) which remains to be determined. To this end, let us
introduce the autocorrelation function of $\delta \beta$,

$$R_{ij}(r) = \langle \delta \beta_{ij}(x) \delta \beta_{kl}(x + r) \rangle. \quad (3.4)$$

But, by virtue of the Wiener-Khinchine theorem, the power spectrum $P(k)$ is the
Fourier transform of the autocorrelation function $R(r)$. Thus, the problem of eval-
uating the sought covariance matrix (3.1) is reduced to that of computing the auto-
correlation function of $\delta \beta$. 
This can be accomplished as follows. Let \( P_2(\delta \beta, \delta \beta' ; x, x') \) be the joint probability of simultaneously observing \( \delta \beta \) at \( x \) and \( \delta \beta' \) at \( x' \). The pointwise distribution of \( \delta \beta \) is denoted by \( P_1(\delta \beta, x) \). Next, we assume statistical homogeneity of the microstructure, whereupon \( P_1 \) can be taken to be independent of \( x \) and \( P_2 \) to depend solely on the relative position vector \( r = x' - x \). Furthermore, if we introduce the ergodic hypothesis that spatial averages can be replaced by statistical expectations, Eq. (3.4) can be recast as

\[
R_{ijkl}(r) = \int \delta \beta_{ij} \delta \beta_{kl} P_2(\delta \beta, \delta \beta' ; r) \ d^4(\delta \beta) \ d^4(\delta \beta').
\]  

(3.5)

At this point, the specific features of the microstructure under consideration need to be brought into the calculations. In particular, we assume that the thermal expansion coefficients of any pair of grains are uncorrelated. To further simplify matters, we take the two-point probabilities to have isotropic form, so that they depend on \( r = |r| \) only. The expected behavior of \( P_2 \) as \( r \to \infty \) is that it tends to \( P_1(\delta \beta)P_1(\delta \beta') \), as befits the assumed lack of correlation between grains. On the other hand, as \( r \to 0 \) \( P_2 \) should tend to \( P_1(\delta \beta)\delta(\delta \beta - \delta \beta') \), in view of the assumed homogeneity of the grains. Note that the Dirac delta function \( \delta(\delta \beta - \delta \beta') \) assigns a vanishing probability to the occurrence of two neighboring points with different thermal properties.

Several models have been proposed in the past for the two-point probabilities of polycrystalline aggregates. For instance, Pekeris (1947) assumed an exponential variation of \( P_2 \) with \( r \), whereas Chernov (1960) advocated the use of an exponential function of \( r^2 \). Other expressions (e.g., Gilbert (1962); Johnson and Mehl (1939); see also Talbot and Willis (1982), for a discussion) have been derived from explicit stochastic cell models. In all cases, the grain size \( a \) sets the characteristic length scale of variation of the two-point correlations.

A particularly simple model consistent with these constraints consists of assuming that

\[
P_2(\delta \beta, \delta \beta' ; r) = \begin{cases} 
P_1(\delta \beta)P_1(\delta \beta') & \text{if } r \geq a; \\
P_1(\delta \beta)\delta(\delta \beta - \delta \beta') & \text{if } r < a.
\end{cases}
\]  

(3.6)

where \( a \) is the radius of the grains. From (3.6) and (3.5) one has

\[
R_{ijkl}(r) = \int \delta \beta_{ij} \delta \beta_{kl} P_1(\delta \beta)P_1(\delta \beta') d^4(\delta \beta) d^4(\delta \beta') = \langle \delta \beta_{ij} \rangle \langle \delta \beta_{kl} \rangle = 0, \quad \text{for } r \geq a
\]  

(3.7)

and

\[
R_{ijkl}(r) = \int \delta \beta_{ij} \delta \beta_{kl} P_1(\delta \beta) d^4(\delta \beta) = \langle \delta \beta_{ij} \delta \beta_{kl} \rangle, \quad \text{for } r < a,
\]  

(3.8)

which can be jointly expressed as

\[
R_{ijkl}(r) = f(r) \langle \delta \beta_{ij} \delta \beta_{kl} \rangle,
\]  

(3.9)

where \( H \) denotes the \( H \) matrix. Recall that the thermal expansion and the \( \mu(Q) \) is a proper orthogonal matrix containing \( \beta \). Since \( P_1(\beta) \) can be reduced to the average value of \( \beta 

where \( \mu(Q) \) denotes a proper orthogonal matrix containing \( \beta \) randomly oriented.

The constant \( C \) can be expressed as

\[
C = \frac{1}{3} \langle \beta_{ij} \rangle \delta_{ij} = \frac{1}{3} \
\]

(3.10)

where use has been made of Eq. (3.14) and the corresponding relations

\[
\delta \beta_{ij}(x) = Q_{ij}(x) \Lambda \delta \beta_{ij}(x)
\]

and

\[
\delta \beta_{ij}(x) = Q_{ij}(x) \Lambda \delta \beta_{ij}(x)
\]

(3.15)

where \( \Lambda \) is the di
he joint probability distribution of $\delta \mathbf{f}$ is the microstructure, depend solely on the ergodic hypothesis, Eq. (3.4) can be expressed as

$$f(r) = 1 - H(r - a)$$

(3.10)

and $H$ denotes the Heaviside step function. Equation (3.9) embodies the assumption that the thermal expansion coefficients are fully correlated within each grain but completely uncorrelated between grains.

In view of (3.9), the problem is now reduced to determining the covariance matrix $\langle \delta \beta_i \delta \beta_j \rangle$ of the thermal expansion coefficients. To this end, we start by noting that, $\beta$ being symmetric, it can be expressed as

$$\beta_{ij}(x) = Q_{ik}(x)Q_{jk} \Lambda_{kl},$$

(3.11)

where $\Lambda = \text{diag} (\beta_1, \beta_2, \beta_3)$ is a diagonal matrix containing the principal values of $\beta$ and $Q$ is a proper orthogonal matrix which characterizes the orientation of the grain containing $x$. Since $\Lambda$ is constant and deterministic, the pointwise probability function $P_1(\beta)$ can be reduced to one $P_1(Q)$ pertaining to the distribution of $Q$. Then, the average value of $\beta$ can be computed as

$$\langle \beta_{ij} \rangle = \int Q_{ik}Q_{jk} \Lambda_{kl} P_1(Q) d\mu(Q),$$

(3.12)

where $\mu(Q)$ denotes the element of volume over the group of three-dimensional proper orthogonal matrices. However, by virtue of the assumption that the grains are randomly oriented $\langle \beta \rangle$ must be isotropic, i.e.

$$\langle \beta_{ij} \rangle = C \delta_{ij}. $$

(3.13)

The constant $C$ can be determined from the scalar equation

$$C = \frac{1}{3} \langle \beta_{ij} \rangle \delta_{ij} = \frac{1}{3} \int \delta_{ij} Q_{ik}Q_{jk} \Lambda_{kl} P_1(Q) d\mu(Q)$$

$$= \frac{1}{3} \delta_{ij} \lambda_{kl} \int P_1(Q) d\mu(Q) = \frac{1}{3} \lambda_{kk},$$

(3.14)

where use has been made of the identity $\delta_{ijkl} = \delta_{ij} Q_{ik}Q_{jk}$ and the normalization condition

$$\int P_1(Q) d\mu(Q) = 1.$$  

(3.15)

Using (3.14), Eq. (3.13) becomes

$$\langle \beta_{ij} \rangle = \frac{1}{3} \lambda_{kk} \delta_{ij} = \frac{\beta_1 + \beta_2 + \beta_3}{3} \delta_{ij}$$

(3.16)

and the corresponding fluctuation field

$$\delta \beta_{ij}(x) = Q_{ik}(x)Q_{jk}(x) \Lambda_{kl} - \langle \beta_{ij} \rangle = Q_{ik}(x)Q_{jk}(x) \Lambda_{kl}$$

$$- \frac{1}{3} \lambda_{kk} \delta_{ij} = Q_{ik}(x)Q_{jk}(x) \Lambda_{kk},$$

(3.17)

where $\Lambda'$ is the deviator of $\Lambda$. It is interesting to note that if the thermal expansion
coefficients are isotropic then \( \Lambda' \) vanishes identically, together with all the fluctuation fields.

From (3.17), the covariance matrix of \( \delta \beta \) is found to be

\[
\langle \delta \beta_{ij} \delta \beta_{kl} \rangle = \int Q_m Q_p \Lambda_{mm} Q_{kp} Q_{pq} P_1(Q) \, d\mu(Q).
\]

But appealing once more to the overall isotropy of the polycrystalline ensemble, one concludes that \( \langle \delta \beta_{ij} \delta \beta_{kl} \rangle \) must be an isotropic tensor, i.e.

\[
\langle \delta \beta_{ij} \delta \beta_{kl} \rangle = A \delta_{ij} \delta_{kl} + B (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}).
\]

(3.19)

The coefficients \( A \) and \( B \) in this expression can be determined by forming the scalars

\[
\langle \delta \beta_{ij} \delta \beta_{kl} \rangle \delta_{ij} \delta_{kl} = 9A + 6B, \quad \langle \delta \beta_{ij} \delta \beta_{kl} \rangle \delta_{ik} \delta_{jl} = 3A + 12B.
\]

(3.20)

From (3.18), the left hand sides in these equations are computed to be

\[
\langle \delta \beta_{ij} \delta \beta_{kl} \rangle \delta_{ij} \delta_{kl} = \int \delta_{ij} \delta_{kl} Q_m Q_p \Lambda_{mm} Q_{kp} Q_{pq} P_1(Q) \, d\mu(Q) = (\Lambda_{kk})^2 \int P_1(Q) \, d\mu(Q) = 0,
\]

\[
\langle \delta \beta_{ij} \delta \beta_{kl} \rangle \delta_{ik} \delta_{jl} = \int \delta_{ik} \delta_{jl} Q_m Q_p \Lambda_{mm} Q_{kp} Q_{pq} P_1(Q) \, d\mu(Q)
\]

\[
= (\Lambda_{ij} \Lambda_{ij}) \int P_1(Q) \, d\mu(Q) = 2b^2,
\]

(3.21)

where one writes

\[
\beta_c = \sqrt{\frac{1}{2} \Lambda_{ij} \Lambda_{ij}} = \sqrt{\frac{1}{2} \beta_{ij} \beta_{ij}},
\]

(3.22)

This parameter can be regarded as a scalar measure of the degree of anisotropy of the grains. Using the relation between \( \beta \) and the thermal expansion tensor \( \alpha \), one finds

\[
\beta_c = \mu \alpha_c, \quad \alpha_c = \sqrt{2x_c x_c},
\]

(3.23)

where \( x_c \) plays the role of an effective thermal expansion coefficient. A minor computation yields the useful identities

\[
\alpha_c^2 = \frac{2}{3} [(\alpha_1 - \alpha_2) + (\alpha_1 - \alpha_3) + (\alpha_2 - \alpha_3)],
\]

\[
\beta_c^2 = \frac{1}{6} [(\beta_1 - \beta_2) + (\beta_1 - \beta_3) + (\beta_2 - \beta_3)].
\]

(3.24)

Solving for \( A \) and \( B \) and substituting into (3.19) we find

The role of grain...
Microstructural thermal stresses in ceramic materials

\[ \langle \delta \beta_{ij} \delta \beta_{kl} \rangle = \frac{\mu^2 \chi^2}{5} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl} \right). \quad (3.25) \]

The role of grain anisotropy in the generation of residual stresses is apparent from this expression. In particular, as already mentioned, it is seen that if the grains are isotropic, i.e. if \( \beta_1 = \beta_2 = \beta_3 \), then the covariance matrix of \( \delta \beta \) and, hence, of \( \delta \sigma \) vanish identically. This latter occurrence in turn implies the absence of residual stresses.

Substitution of (3.25) and (3.9) into (3.2) yields the sought expression for the covariance matrix of the residual stresses, namely

\[ \langle \delta \sigma_{ij} \delta \sigma_{kl} \rangle = \frac{\mu^2 \chi^2 \theta^2}{5} \left( \delta_{mp} \delta_{na} + \delta_{mp} \delta_{np} - \frac{2}{3} \delta_{mn} \delta_{pq} \right) \int A^*_{ijmn}(k) A_{klpq}(k) f(k) \, d^3 k. \quad (3.26) \]

The computation of this integral expression is greatly simplified by noting that the outcome must be an isotropic tensor, by virtue of the overall isotropy of the body. Then, proceeding as in (3.20) and after lengthy but straightforward computations one finds

\[ \langle \delta \sigma_{ij} \delta \sigma_{kl} \rangle = p(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) - q \delta_{ij} \delta_{kl}, \quad (3.27) \]

where the coefficients \( p \) and \( q \) are given by

\[ p = \mu^2 \chi^2 \theta^2 \frac{46 v^2 - 88 v + 46}{225(1 - v)^2}, \quad q = \mu^2 \chi^2 \theta^2 \frac{24 v^2 - 72 v + 24}{225(1 - v)^2}. \quad (3.28) \]

We note that in deriving (3.27) and (3.28) use has been made of identity (41.2b) and the fact that, as is apparent from (3.10), \( f(0) = 1 \).

Equations (3.27) and (3.28) constitute the main result of this paper. It is interesting to note that the distribution of residual stresses is determined by the temperature drop \( \theta \), the degree of anisotropy as measured by \( \chi \), and the elastic moduli. The grain size drops out of the results, a direct manifestation of the absence of a characteristic length in the problem. By contrast, the extent of microcracking is known to be strongly dependent on the grain size, as pointed out by numerous authors (Kuszyk and Bradt, 1973; Dole et al., 1976; Pohanka et al., 1976; Siebenek et al., 1976; Cleveland and Bradt, 1978). In this case, the length scale is set by the toughness of the grain facets.

4. Application to Spontaneous Microfracture

A first-order estimate of the extent of thermally induced microcracking can be readily derived from the results of the preceding section. Thus, from (3.27), it is possible to determine the probability distribution of normal stresses acting on grain facets. Then, the density of microcracks follows by recourse to the simplifying assumption that nucleation is governed by a critical normal stress.
We start by assuming that the residual stresses are normally distributed. Thus, the probability density function of $\delta \sigma$ is entirely determined by the covariance matrix (3.27) and takes the form

$$P(\delta \sigma) = \frac{\det(M)^{1/2}}{(2\pi)^{3/2}} \exp \left( -\frac{1}{2} M_{ijkl} \delta \sigma_i \delta \sigma_k \right),$$

(4.1)

where $M_{ijkl} = \langle \delta \sigma_i \delta \sigma_k \rangle^{-1}$. Note that, by isotropy, $P(\delta \sigma)$ is expressible in terms of the principal values of $\delta \sigma$ alone. Another consequence of isotropy is that the distribution $P(\delta \sigma_n)$ of normal stresses $\delta \sigma_n$ is independent of the orientation of the plane on which they act. Thus, we can identify $P(\delta \sigma_n)$ with the distribution of, say, $\delta \sigma_{11}$. From general properties of multivariate normal distributions (see, e.g., FELLER, 1971) it follows that $P(\delta \sigma_n)$ is itself normal, i.e.

$$P(\delta \sigma_n) = \frac{1}{\sqrt{2\pi} \sigma} \exp \left( -\frac{\delta \sigma_n^2}{2\sigma^2} \right),$$

(4.2)

where the covariance $\sigma$ is computed from (3.27) and (3.28) to be

$$\sigma^2 = \langle \delta \sigma_{11} \delta \sigma_{11} \rangle = 2p - q = \mu^2 \alpha^2 \theta^2 g^2(v), \quad g^2(v) = \frac{68v^2 - 104v + 68}{225(1-v)^2}.$$
distributed. Thus, the covariance matrix

$$
\begin{align}
\mathbf{C} = \sum_{i,j} \mathbf{R}_{ij} \mathbf{S}_{ij}
\end{align}
$$

(4.1)

emissible in terms of py is that the distation of, say, \( \delta \sigma_{11} \), e.g., FELLER, 1971)

$$
\begin{align}
104v + 68 \\
(1-v)^2
\end{align}
$$

(4.3)

one that the microion of \( \sigma_e \) from the rest in itself which strong dependence 1982; KRSTIC, 1984; orselly proportional microcracking can

$$
\begin{align}
\text{Critical normal in be computed as}
\end{align}
$$

(4.4)

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$$
\begin{align}
\text{(4.5)}
\end{align}
$$

Microstructural thermal stresses in ceramic materials

![Graph showing fraction of fractured facets as a function of the level of residual stress.]

Fig. 1. First-order estimate of fraction of fractured facets as a function of the level of residual stress.

$$
\begin{align}
\frac{f(\sigma/\sigma_e)}{\sigma_e} \sim \frac{1}{2\pi} \frac{\sigma}{\sigma_e} \exp \left( -\frac{\sigma_e^2}{2\sigma^2} \right)
\end{align}
$$

(4.6)

This function is shown in Fig. 1. As can be seen, the fraction of fractured facets is negligibly small for values of \( \sigma \) below \( \sigma_e/2 \), increasing sharply thereafter. Thus, the extent of microcracking can be expected to be very sensitive to the value of \( \sigma_e \) and, hence, to the grain size.

A question of some interest concerns the range of validity of the linear analysis given in Sections 2 and 3, which regards the body as being essentially intact. This issue can be ascertained by examining the extent to which the elastic moduli are affected by microcracking during a typical cooling process. A measure of microcrack density which arises naturally in Budiansky and O'Connell's self-consistent treatment of microfractured solids is defined by

$$
\begin{align}
\varepsilon = 2\rho/\pi \left\langle A^2/P \right\rangle,
\end{align}
$$

(4.7)

where \( \rho \) is the number of microcracks per unit volume, and \( A \) and \( P \) denote the area and perimeter of the microcracks. For circular microcracks of radius \( R \), \( \varepsilon \) reduces simply to \( \rho \left\langle R^2 \right\rangle \). From estimates derived in Appendix 2 one draws the relation

$$
\begin{align}
\varepsilon = \frac{3}{\pi \sqrt{n}} f
\end{align}
$$

(4.8)

where \( n \) is the number of facets per grain. This latter quantity has been determined to range from nine to eighteen. A shape which is sometimes assumed for three dimensional grains is that of a tetrakaidecahedra (KINGERY et al., 1976), which comprises six square and eight hexagonal faces, giving \( n = 14 \). For this value of \( n \), (4.8) becomes \( \varepsilon \approx 0.255 f \).

Equation (4.8) combined with (4.6) can be utilized to determine the variation of the elastic moduli induced by microcracking. To this end, we resort to the self-consistent estimates of Budiansky and O'Connell. In particular, the effective Young's modulus \( E \) is well approximated by the expression
\[ E \approx (1 - 16\varepsilon /9)E. \]

(4.9)

To obtain a feel for the degree of nonlinearity introduced by microcracking, we investigate the case of Al$_2$O$_3$. For this material Kingery et al. (1976) give: 
\[ E = 3.8 \times 10^5 \text{ MPa, } v = 0.25, \alpha_1 = \alpha_2 = 8.3 \times 10^{-6} \text{ °C}^{-1}, \alpha_3 = 9.0 \times 10^{-6} \text{ °C}^{-1}, \text{ and } \gamma = 0.905 \text{ J/m}^2. \]
For these values \( \alpha_1 = 0.81 \times 10^{-6} \text{ °C}^{-1}, \mu = 1.52 \times 10^5 \text{ MPa and } \eta(\nu) = 0.60. \) Assuming a temperature drop \( \theta = 1500^\circ \text{C}, \) the variance of the normal tractions is computed to be \( \sigma = 110 \text{ MPa}. \) Note that the temperature drop is measured from a loosely defined effective solidification temperature above which the stresses in the sample rapidly relax due to creep, and below which no relaxation occurs. Most authors have assumed this temperature to be independent of the grain size and the cooling rate (Kuszyk and Bradt, 1973; Cleveland and Bradt, 1978; Evans, 1978; Rice and Pohanka, 1979; Case et al., 1980; Rice and Freiman, 1981). Using spectroscopic \( R \) lines, Blendell and Coble (1982) estimated the magnitude of the thermal stresses in alumina to be in the range 80–100 MPa. The agreement is not unreasonable in view of the uncertainties involved in the experimental measurements (±30%) and in the values of the material constants employed in the computations.

The computed magnitude of the thermal stresses is capable of causing moderate amounts of microcracking for sufficiently large grain sizes. Thus, using the rough estimate (4.27) for \( \sigma_0, \) derived in Appendix 2, we obtain the values \( \sigma_0 = 569, 402, 180 \) and 127 MPa for \( a = 5, 10, 50 \) and 100 \( \mu \text{m}, \) respectively. The extent of microfracturing is negligible for the two smallest grain sizes. For \( a = 50 \) and 100 \( \mu \text{m} \) one obtains \( f = 2.5\% \) and 7.1\%, and, from (4.8) and (4.9), \( \bar{E} = 0.989E \) and \( \bar{E} = 0.968E, \) respectively. As can be seen, the reduction in Young’s modulus is sufficiently small that the linear theory can be reasonably expected to remain valid. For larger grain sizes, the extent of microcracking increases sharply and the linear analysis no longer applies.

ACKNOWLEDGEMENTS

MO gratefully acknowledges the support of the Office of Naval Research through grant N00014-85-K-0720.

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APPENDIX 1
GENERAL RESULTS FROM FOURIER ANALYSIS

Some basic properties of the Fourier transform are recorded next. The Fourier transform
of a function \( f(x) \) of the spatial coordinates \( x \equiv (x_1, x_2, x_3) \) is defined as

\[
\hat{f}(k) = \int f(x)e^{-kx} \, d^3x.
\]  

(A1.1)

The following standard results are used throughout the paper.
\[ \langle f(y) \rangle = \lim_{V \to \infty} \frac{1}{V} \int f^*(k) g_V(k) \, d^3 k, \]

\[ f(0) = \int f(k) \, d^3 k. \tag{A1.2} \]

In the first identity, \( f^* \) and \( g_V \) signify the restrictions of \( f \) and \( g \) to a closed compact subset \( V \) of \( \mathbb{R}^3 \) containing the origin. In terms of the limiting process indicated in the first of \( (A1.2) \), \( f^* \) and \( g_V \) are to be regarded as members of two nets of functions obtained by letting the domain \( V \) cover the whole space. For example \( V \) can be taken to be the ball of radius \( R \) centered at the origin and the limit in \( (A1.2) \) reduces to letting \( R \to \infty \). It is implicitly assumed that due to statistical disorder the result is independent of the choice of origin. For simplicity of notation, the subindex \( V \) in the integrand of \( (A1.2) \) is dropped throughout the paper.

**APPENDIX 2**

**ESTIMATES OF \( \varepsilon \) AND \( \sigma_\varepsilon \)**

In order to compute \( \varepsilon \) we need to estimate the parameters \( \rho \) and \( R \). The former takes the form \( \rho = f \rho_f \), where \( \rho_f \) is the number of facets per unit volume. Let us assume that the grains are of uniform volume \( V_g \) and that each grain has \( n \) facets. Then, \( \rho_f \) is given by \( \rho_f = n / V_g \).

Taking \( V_g \approx 4\pi a^3 / 3 \), \( a \) being the radius of the grains, we obtain

\[ \rho = \frac{3n}{8\pi a^3} f. \tag{A2.1} \]

If we further assume that the facets are of uniform area \( A_f \), we have \( A_f \approx 4\pi a^2 / n \), and taking \( A_f \approx \pi R^2 \), \( R \) being the radius of the facets, we obtain a relation

\[ R = \frac{2a}{\sqrt{n}}. \tag{A2.2} \]

Substituting \( (A2.1) \) and \( (A2.2) \) into \( (4.7) \), we arrive at the sought result

\[ \varepsilon = \frac{3}{\pi \sqrt{n}} f. \tag{A2.3} \]

Next, we turn our attention to the estimation of \( \sigma_\varepsilon \). A rigorous calculation of this quantity would necessitate a detailed investigation of the mechanics of a plausible microcrack nucleation mechanism. Here, however, the aim is to obtain a rough estimate of \( \sigma_\varepsilon \), which permits determining its order of magnitude from commonly available experimental data. We start by recalling that the strain energy released by the opening of a circular crack of radius \( R \) subjected to remote normal stress \( \sigma_n \) is (see, e.g., Sneddon, 1969)

\[ \varepsilon = \frac{8(1 - v^2)R^3}{3E} \sigma_n^2. \tag{A2.4} \]

The energy required to create the new surface can be estimated as

\[ \mathcal{S} = 2 \gamma \pi R^2, \tag{A2.5} \]

where \( \gamma \) is the surface energy of the grain facet. Finally, establishing a balance of energy \( \varepsilon = \mathcal{S} \), we find

\[ \sigma_\varepsilon = \sqrt{\frac{3\pi E \gamma}{4(1 - v^2)R^2}}, \tag{A2.6} \]

The critical stress \( \sigma_\varepsilon \) can be related to the grain size with the aid of \( (A2.2) \), which yields

**EFFECTS OF...**

In this Appendix we study microstructural elastic and first approximation. Numerical results of far-reaching have shown that elastic interactions between grains are often, thus

For the purpose of simplicity of stress potentials. Equations, potentials \( \chi_j \) (Kroner, 1)

The strain field, on the other hand, is

Finally, we rephrase Eq. \( \eta \), where \( C \) are the elastic coefficients exhibit micro

which is to be solved for

Next, we envision a heterogeneous, respectively, and introduce

where \( \mathcal{C} \) and \( \mathcal{\tilde{a}} \) are some

The functions \( \chi_1 \) and \( \gamma \) are heterogeneity, respectively, and found from \( (A3.4) \) and

The first equation corresponds to Under these conditions second of \( (A3.7) \) reduc
Microstructural thermal stresses in ceramic materials

\[ \sigma_c = \frac{3\pi E_1 \sqrt{n}}{8(1 - v^2)a} \]  \hspace{1cm} (A4.7)

The energy balance concept underlying this simple estimate has been utilized by numerous authors (Clarke, 1964; Davidge and Green, 1968; Kuszyk and Bradt, 1973; Cleveland and Bradt, 1978; Evans, 1978) to determine a critical grain size for spontaneous cracking due to thermal expansion anisotropy.

\section*{Appendix 3}
\textbf{Effect of Elastic Anisotropy on Thermal Stresses}

In this Appendix we show that, for small deviations from homogeneity, the influence of the microstructural elastic anisotropy is a second-order effect and can therefore be neglected to a first approximation. Note, however, that elastic anisotropy may produce local stress fluctuations of far-reaching consequences. Thus, for instance, Hutchinson and Tvergaard (1987) have shown that elastic anisotropy strongly influences conditions at triple point junctions between grains and, thus, may significantly affect the process of microcrack nucleation.

For the purpose of this discussion, it proves advantageous to formulate the problem in terms of stress potentials. Equilibrium is identically satisfied by deriving the stress field from a stress potential \( \psi \) (Kroner, 1960; see also Ortiz, 1987):

\[ \sigma_{ij} = (\nabla \times \chi \times \nabla)_{ij} = e_{mn,kl} e_{ikm} e_{ijn}. \]  \hspace{1cm} (A3.1)

The strain field, on the other hand, must satisfy the compatibility equation

\[ (\nabla \times \epsilon \times \nabla)_{ij} = e_{mn,kl} e_{ikm} e_{ijn} = 0. \]  \hspace{1cm} (A3.2)

Finally, we rephrase Eq. (2.1) as

\[ \epsilon_{ij} = C_{ijkl} \sigma_{kl} + a_{ij} \theta, \]  \hspace{1cm} (A3.3)

where \( C \) are the elastic compliances and \( \theta \) is the thermal expansion tensor. Combining the above equations, we obtain

\[ \nabla \times [C : (\nabla \times \chi \times \nabla) + a \theta] \times \nabla = 0 \]  \hspace{1cm} (A3.4)

which is to be solved for the stress potential \( \chi \).

Next, we envisage a solid in which both the elastic moduli and the thermal expansion coefficients exhibit microstructural heterogeneity. Let us adopt the representation

\[ C(x) = \tilde{C} + \epsilon_1 \delta \tilde{C}(x), \quad \chi(x) = \tilde{\chi} + \epsilon_2 \delta \chi(x), \]  \hspace{1cm} (A3.5)

where \( \tilde{C} \) and \( \tilde{\chi} \) are some effective values of the elastic moduli and thermal expansion coefficients, respectively, and introduce a perturbation expansion of \( \chi \) of the form

\[ \chi = \chi_0 + \epsilon_1 \chi_1 + \epsilon_2 \chi_2 + \cdots. \]  \hspace{1cm} (A3.6)

The functions \( \chi_1 \) and \( \chi_2 \) constitute the first-order corrections to \( \chi_0 \) due to elastic and thermal heterogeneity, respectively. The equations governing these terms of the expansion are readily found from (A3.4) and (A3.5) to be

\[ \nabla \times [C : (\nabla \times \chi_0 \times \nabla) + \tilde{\chi} \theta] \times \nabla = 0, \]
\[ \nabla \times [C : (\nabla \times \chi_1 \times \nabla) + \delta C : (\nabla \times \chi_0 \times \nabla)] \times \nabla = 0, \]
\[ \nabla \times [C : (\nabla \times \chi_2 \times \nabla) + \delta \chi \theta] \times \nabla = 0, \]
\[ \cdots \]  \hspace{1cm} (A3.7)

The first equation corresponds to a homogeneous body undergoing uniform thermal expansion. Under these conditions, no stresses are generated and \( \chi_0 = 0 \). Making use of this result, the second of (A3.7) reduces to

\[ \nabla \times [C : (\nabla \times \chi_1 \times \nabla)] \times \nabla = 0. \]
which yields \( \chi = 0 \). Thus it is concluded that, to within first-order terms, elastic anisotropy has no effect on the thermal stresses. The first non-trivial term in the expansion is furnished by the third of (A3.7), which determines the state of stress in an elastically homogeneous body with heterogeneous thermal expansion coefficients subjected to a uniform temperature variation. This is precisely the problem investigated in the body of the paper. 

A SIMPLE numerical sche involving rigid indenters of pressure to the given disp to a system of algebraic for the pressure. Results and normal surface displ circular indenters for \( \beta \in 0 \leq \beta \leq 0.5. \)

\begin{align*}
    a & \quad \text{contact rad} \\
    a_R & \quad (3\pi R^4/4) \\
    E & \quad \text{Young's m} \\
    K & \quad \text{complete c} \\
    J_0 & \quad \text{Bessel func} \\
    p(r) & \quad \text{pressure at} \\
    p(0) & \quad \text{pressure at} \\
    P & \quad \text{load on in} \\
    R & \quad \text{radius of a} \\
    t & \quad \text{layer thick} \\
    (r, z) & \quad \text{cylindrical} \\
    (u, v) & \quad \text{displacem} \\
    a & \quad 1 - \nu^2/E \\
    \beta & \quad a/r \\
    v & \quad \text{Poisson's r} \\
    (\sigma_{zz}, \sigma_{rr}) & \quad \text{normal an} \\
\end{align*}

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