

# MATERIAL FORCE MODELS FOR CRACKS - INFLUENCES OF EIGENSTRAINS, THERMAL STRAINS & RESIDUAL STRESSES

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## ABSTRACT

Eigenstrains, thermal strains and residual stresses can strongly influence the failure behavior of materials and structural components. This paper will develop material forces models for evaluating their influence on the crack driving force in elastic and elastic-plastic materials.

## 1 INTRODUCTION

The improved fracture toughness of zirconia-toughened ceramics is due to eigenstrains resulting from a crack tip induced phase transformation. Other material systems where eigenstrains play an important role include TRIP steels, TiAl alloys, shape-memory alloys and martensites. Materials and structural components are subject to considerable temperature fluctuations both during fabrication processes and under certain working conditions, hence thermal strains become important whenever components have inhomogeneous thermal properties. Residual stresses are intentionally introduced by specialized treatments like shot peening for enhancing fracture properties of components. Also, eigenstrains and thermal strains are typically accompanied by residual stresses, which in turn will influence cracks.

The material forces approach has seen renewed interest in the past decade (see Simha et al. [1, 2] and references there). Advances include theoretical developments (Gurtin [3], Maugin [4], Kienzler & Hermann [5]) and formulation of novel computational schemes (Steinmann [6], Mueller & Maugin [7], Mueller et al. [8]). Our recent efforts have been focused on understanding the influences of inhomogeneous material properties on crack initiation and growth; material force models and computational schemes were developed, and then applied to comprehensively catalogue inhomogeneity effects in elastic and elastic-plastic materials (Simha et al. [1, 2], Kolednik et al. [9, 10]). There is a strong link between inhomogeneous material properties and the topics – eigenstrains, thermal strains and residual stresses – considered here. For instance, a mismatch in thermal properties at a bimaterial interface will result in residual stresses, which in turn can influence cracks. So by building on the theoretical developments in Simha et al. [1,2], this paper will examine the effects of eigenstrains, thermal strains and residual stresses on the crack driving force in elastic as well as elastic-plastic materials.

## 2 THEORETICAL BACKGROUND

The notion of crack tip shielding or anti-shielding is very useful in understanding the influences of factors such as inhomogeneous material properties, eigenstrains, continuum damage and plastic deformations on crack initiation and growth. The idea is that these factors either shield the crack tip from the nominally applied far-field crack driving force  $J_{far}$ , so the effective near-tip crack driving force  $J_{tip}$  is smaller than  $J_{far}$  or anti-shield by enhancing the effect of the applied  $J_{far}$ , so  $J_{tip}$  is larger than  $J_{far}$ .

The primary result we need is the relation between the effective crack driving force  $J_{tip}$  and the nominally applied far-field driving force  $J_{far}$ . As shown in Simha et al. [1, 2]

$$J_{tip} = J_{far} + C \quad (1)$$

where  $J_{tip}$  and  $J_{far}$  are obtained by evaluating the standard J-integral on contours close to the crack tip and in the far field (Fig. 1a); we call  $C$  the material term, it quantifies the crack tip shielding or anti-shielding, and is given by

$$C = -\mathbf{e} \cdot \int_D \nabla \cdot (\phi \mathbf{I} - \mathbf{F}^T \mathbf{S}) dA - \sum_{i=1}^k \int_{\Sigma^i} ([[\phi]] - \langle \mathbf{S} \rangle \cdot [[\mathbf{F}]]) (\mathbf{n}^i \cdot \mathbf{e}) ds \quad (2)$$

here  $\phi$  is the stored energy density (Helmholtz potential),  $\mathbf{F}$  is the deformation gradient,  $\mathbf{S}$  is the Piola-Kirchhoff stress,  $\mathbf{e}$  is the direction of crack growth,  $\nabla$  is the Lagrangian derivative, the region  $D$  refers to the area between the contours used to evaluate the near-tip and far-field integrals (Fig. 1), there are  $\Sigma^i$ ,  $i=1,2 \dots k$ , sharp interfaces in the region  $D$ ,  $\mathbf{n}^i$  is the unit normal to interface  $\Sigma^i$  and  $[[b]]$  denotes the jump across an interface of a quantity  $b$ , while  $\langle b \rangle$  denotes the average. The area integral in eqn (2) is taken only over the areas inside region  $D$  excluding the  $k$  interfaces. If the material term  $C$  is negative, then it shields the tip from the applied far-field driving force, whereas if it is positive it enhances the applied driving force and hence results in anti-shielding. Alternately, suppose that the crack grows when the crack tip driving force reaches a critical value, i.e.  $J_{tip} \geq J_c$ . Note that (1) implies that  $J_{far} \geq J_c - C$ . So, if  $C < 0$ , then the applied driving force needs to exceed the critical value for crack growth; in contrast if  $C > 0$  the crack can grow even when  $J_{far}$  is smaller than  $J_c$ .

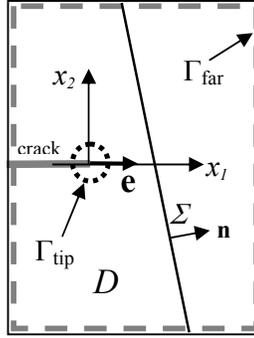


Figure 1. A two dimensional body containing a crack growing along direction  $\mathbf{e}$  and a sharp interface  $\Sigma$  with unit normal  $\mathbf{n}$ .  $J_{tip}$  is evaluated on contour  $\Gamma_{tip}$ , while  $J_{far}$  is evaluated on  $\Gamma_{far}$ ;  $D$  is the region between the two contours.

Simha et al. [1, 2] do not assume the materials to be nonlinear elastic for deriving eqns (1) and (2), hence these are valid for a wider class of materials. We next suppose that the stored energy density  $\phi = \phi(\mathbf{F}, \mathbf{x})$  where  $\mathbf{x}$  denotes the reference coordinate. The dependence on the deformation gradient  $\mathbf{F}$  is relevant for elastic and (rate-independent) elastic-plastic materials, whereas we will show below that the explicit dependence on the reference coordinate can account for eigenstrains, thermal strains and residual stresses. For this type of stored energy, the integrand of the first integral in eqn (2) simplifies (Simha et al. [1]), and the material term can be written as

$$C = -\mathbf{e} \cdot \int_D \frac{\partial \phi(\mathbf{F}, \mathbf{x})}{\partial \mathbf{x}} dA - \sum_{i=1}^k \int_{\Sigma^i} ([[\phi]] - \langle \mathbf{S} \rangle \cdot [[\mathbf{F}]]) (\mathbf{n}^i \cdot \mathbf{e}) ds \quad (3)$$

It is important to note that the derivative is with respect to the reference coordinate  $\mathbf{x}$  and is taken while holding  $\mathbf{F}$  fixed. When the body does not contain any sharp interfaces the second integral vanishes; in

addition, if the material is homogeneous the first integral vanishes, the material term  $C=0$ . This essentially recovers the path independence of the J-integral for nonlinear elasticity and deformation plasticity.

Next, for the linear setting,  $\boldsymbol{\varepsilon}$  denotes the linear elastic strain, the stored energy is taken to be  $\phi=\phi(\boldsymbol{\varepsilon}, \mathbf{x})$ , the Cauchy stress  $\boldsymbol{\sigma}$  is given by  $\boldsymbol{\sigma}(\mathbf{x})=\partial\phi(\boldsymbol{\varepsilon}, \mathbf{x})/\partial\boldsymbol{\varepsilon}$ , and eqn (3) becomes

$$C = -\mathbf{e} \cdot \int_D \frac{\partial\phi(\boldsymbol{\varepsilon}, \mathbf{x})}{\partial\mathbf{x}} dA - \sum_{i=1}^k \int_{\Sigma^i} (\llbracket\phi\rrbracket - \langle\boldsymbol{\sigma}\rangle \cdot \llbracket\boldsymbol{\varepsilon}\rrbracket) (\mathbf{n}^i \cdot \mathbf{e}) ds. \quad (4)$$

In terms of Cartesian components, the material term can be written as

$$C = -e_j \int_D \frac{\partial\phi(\varepsilon_{pq}, x_p)}{\partial x_j} dA - \sum_{i=1}^k \int_{\Sigma^i} (\llbracket\phi\rrbracket - \langle\sigma_{pq}\rangle \llbracket\varepsilon_{pq}\rrbracket) (n_j^i e_j) ds. \quad (5)$$

Note that the derivative in the first integral is taken in the direction of crack growth while the second integral contains the jump in the Eshelby tensor along the direction of crack growth.

### 3 EIGENSTRAINS

The total strain  $\boldsymbol{\varepsilon}$  is now split into the elastic part  $\boldsymbol{\varepsilon}^e$  and the eigenstrain  $\boldsymbol{\varepsilon}^*$ . The eigenstrain is determined by phenomena like phase transformation and is taken to be independent of the elastic strain. We account for eigenstrains by taking the stored energy to be  $\phi=\phi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^*(\mathbf{x}))$ ; now the dependence on the reference coordinate is through the eigenstrain. Then

$$\frac{\partial\phi(\varepsilon_{pq}, \varepsilon_{pq}^*(x_p))}{\partial x_j} = \frac{\partial\phi}{\partial\varepsilon_{pq}^*} \bigg|_{\varepsilon_{pq}} \frac{\partial\varepsilon_{pq}^*(x_p)}{\partial x_j}. \quad (6)$$

Further simplifications follow if we adopt the following specific form

$$\phi = (K_{ijkl} / 2) \varepsilon_{ij}^e \varepsilon_{kl}^e \quad \text{where} \quad \varepsilon_{ij}^e = \varepsilon_{ij} - \varepsilon_{ij}^* \quad \text{and} \quad \sigma_{ij} = K_{ijkl} \varepsilon_{kl}^e \quad (7)$$

where  $K_{ijkl}$  denotes the linear elastic moduli. These expressions are commonly used in micromechanics, e.g. Mura [11]. Then the derivative with respect to the eigenstrain can be calculated and eqn (6) becomes

$$\frac{\partial\phi}{\partial\varepsilon_{pq}^*} \bigg|_{\varepsilon_{pq}} = -\sigma_{pq}, \quad \text{so} \quad \frac{\partial\phi}{\partial x_j} = -\sigma_{pq} \frac{\partial\varepsilon_{pq}^*}{\partial x_j}.$$

Next, we simplify the integrand of the second integral in eqn (5). Using expressions (7), the identity  $\llbracket\llbracket ab \rrbracket\rrbracket = \llbracket\llbracket a \rrbracket\rrbracket \langle b \rangle + \langle a \rangle \llbracket\llbracket b \rrbracket\rrbracket$  and symmetry of the elastic moduli, a direct calculation shows that

$$\llbracket\llbracket\phi\rrbracket\rrbracket - \langle\sigma_{pq}\rangle \llbracket\llbracket\varepsilon_{pq}\rrbracket\rrbracket = -\langle\sigma_{pq}\rangle \llbracket\llbracket\varepsilon_{pq}^*\rrbracket\rrbracket.$$

Consequently, the material term due to a field of eigenstrains  $\varepsilon_{pq}^* = \varepsilon_{pq}^*(x_p)$  is given by

$$C = e_j \int_D \sigma_{pq} \frac{\partial \varepsilon_{pq}^*}{\partial x_j} dA + \sum_{i=1}^k \int_{\Sigma^i} \langle \sigma_{pq} \rangle \llbracket \varepsilon_{pq}^* \rrbracket (n_j^i e_j) ds \quad (8)$$

The first integral accounts for a smooth distribution, while the second accounts for sharp interfaces.

#### 4 THERMAL STRAINS

Thermal strains can be treated as a special type of eigenstrain. The strain due to temperature changes does not have a shear component and contributes only to normal strains,

$$\varepsilon_{pq}^* = \alpha \Delta T \delta_{pq} \quad (9)$$

where  $\alpha$  is the coefficient of thermal expansion,  $\Delta T$  is the temperature change (current-initial) and  $\delta_{ij}$  is the Kronecker Delta function. Then, the material term due to thermal strains is obtained from (8) as

$$C = e_j \int_D \sigma_{pp} \frac{\partial \alpha}{\partial x_j} \Delta T dA + \sum_{i=1}^k \int_{\Sigma^i} \langle \sigma_{pp} \rangle \llbracket \alpha \rrbracket \Delta T (n_j^i e_j) ds \quad (10)$$

The first integral accounts for smooth inhomogeneities in the thermal coefficient, while the second accounts for discontinuous jumps at sharp bimaterial interfaces or phase boundaries. In general, the temperature field is obtained by solving a heat transfer problem, however in this context all that is needed are the current and initial temperatures. Also it is reasonable to assume that the temperature is continuous at bimaterial interfaces and phase boundaries. Temperature gradients can be present in a cracked body, however such gradients are Eulerian. Since the derivative in the first integral in (10) is Lagrangian, the derivative of temperature does not appear in eqn (10). Thus temperature gradients do not directly contribute to the material term. However, temperature can alter plastic parameters like the yield stress, and such inhomogeneities in material properties will contribute to the material term  $C$  (Simha et al. [1, 2]).

#### 5 RESIDUAL STRESSES

An important aspect of eigenstrains is that they can be accompanied by residual stress fields, so we now discuss methods to quantify the influence of residual stresses on cracks. Since thermal strains are simpler to understand than eigenstrains, we use it to explain important points. First, the existence and magnitude of thermal strains are controlled by temperature. Second, thermal strains result in residual stresses only if constrained, since a homogeneous body that is unconstrained will simply undergo changes in dimensions freely. Finally, residual fields can exist even in the absence of externally applied mechanical loads.

A simple constraint is a bimaterial interface where the material with the smaller thermal coefficient  $\alpha$  will restrict the expansion of the material with higher  $\alpha$ . Consequently, the stresses and strains on either sides of the interface will not vanish. The influence of such a residual field on any cracks in the vicinity can be estimated from the second term in eqns (3) and (4). A second example would be a composite containing a varying volume fraction of small second phase inclusions that have a thermal coefficient different from the matrix. On the macroscopic scale of the composite, the varying volume fraction translates to a varying effective thermal coefficient. Since each inclusion is constrained by the matrix, temperature changes will result in a residual stress field. The influence of such a residual field can be evaluated from the first term of eqns (3) and (4). The bimaterial interface example is examined in detail in a companion paper in these proceedings (Rakin et al. [12]).

The general case of eigenstrains is similar to that of thermal strains with primarily one additional complexity. This is because the existence and magnitude of eigenstrains may also depend upon stresses or strains, and in general it is difficult to compute the magnitude of eigenstrains (see e.g. Fischer et al.

[13]). However, once the eigenstrains are known, the situation is exactly like that of thermal strains – constraints are required to produce residual stresses and these can exist in the absence of externally applied mechanical loads. In the crack shielding or anti-shielding framework specified by eqns (1) and (2), the effects of such residual stress fields on cracks in the vicinity can only be evaluated indirectly through the eigenstrains. In the linear setting, the material term is obtained from eqn (8), where the first term corresponds to continuous distributions of eigenstrains, while the second is for jumps.

## 6 DISCUSSION AND CONCLUSIONS

The focus of this paper is to provide expressions to quantify the influences of eigenstrains, thermal strains and residual stresses on the crack driving forces. It is convenient to characterize such influences in terms of crack tip shielding or anti-shielding, which in turn are quantified by the material term  $C$ . The material term due to eigenstrains, thermal strains, residual stresses (as well as inhomogeneous material properties) is given in general by eqn (3) for the finite strain setting and by eqn (4) for the small strain setting. In this setting, the crack tip shielding and anti-shielding due to residual stresses are evaluated indirectly via the corresponding eigenstrains.

The general expression (4) for the crack tip shielding or anti-shielding can be specialized to obtain eqn (8) for eigenstrains and eqn (10) for thermal strains. These specialized forms are especially useful for analytical calculations.

In a computational framework, the material term can be evaluated by post-processing, after equilibrium stress and strain fields have been evaluated (Simha et al. [2]). Computational packages like ABAQUS ([www.abaqus.com](http://www.abaqus.com)) provide standard methods to evaluate the J-integral, and in Simha et al. [2] we have shown that this can be adapted to accurately evaluate the surface integral in equation (4). However, at present, custom post-processors are required to evaluate the volume integral in eqns (4), (8) and (10). Since a standard method is available to evaluate the surface integral in (4), it is simpler to work with this than with the specialized versions in eqns. (8) and (10) (Rakin, et al. [12]).

Residual stresses can result in crack tip shielding or anti-shielding even in the absence of externally applied mechanical loads. Quantitative results are provided in a companion paper (Rakin et al. [12]).

In conclusion, this paper provides a framework for evaluating the effects of eigenstrains, thermal strains and residual stresses. In Simha et al. [1, 2], we have recently developed robust accurate methods for evaluating the effects of inhomogeneous material properties. Together, these provide a comprehensive framework for studying and developing new methods to enhance the fracture and fatigue properties of materials and structural components.

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