 ANALYSIS OF TOUGHENING OF MAGNESIA PARTIALLY STABILIZED ZIRCONIA, DUE TO DILATATIONAL TRANSFORMATION

H. OKADA¹, T. TAMURA¹, N. RAMAKRISHNAN¹, S. N. ATLURI¹ and J. S. EPSTEIN²

¹Computational Modeling and Infrastructure Rehabilitation Center, Georgia Institute of Technology, Atlanta, GA 30332-0356 and ²Fracture Behavior Group, Idaho National Engineering Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-2218, U.S.A.

(Received 24 June 1991)

Abstract—An analysis of toughening of magnesia partially stabilized zirconia (Mg-PSZ) due to dilatational transformation is presented in this paper. Transformation toughening of Mg-PSZ is attributed to the stress-induced phase transformation of tetragonal zirconia to monoclinic structure in the neighborhood of a macro-crack tip. A rate (incremental) type constitutive model is developed, using a micromechanics approach, wherein the interaction between a transformed zirconia particle and the rest of the material is considered. Problems of stationary and stably propagating cracks are analyzed, using a finite element method. The results of finite element analysis are compared to those of an experimental study by Perry et al. In the comparison, it is found that the displacement field and toughness enhancement during stable crack propagation, predicted by the finite element analysis, are very analogous to those obtained in the experimental study. Moreover, the present constitutive model is capable of revealing detailed information, such as the distribution of transformed zirconia in the wake zone.

Résumé—Dans cet article on présente une analyse de la ténacité d’une zircone partiellement stabilisée par la magnésie (Mg-PSZ) à la suite d’une transformation par dilatation. La ténacité de transformation du Mg-PSZ est attribuée à la transformation de phase, induite par la contrainte, de la zircone quadratique à une structure monoclinique au voisinage de l’extrémité d’une maro fissure. On développe un modèle de vitesse (incrémental) qui utilise une approche micromécanique où l’on considère l’interaction entre une particule de zircone transformée et le reste du matériau. Les problèmes de fissures stationnaires et de fissures se propageant d’une manière stable sont analysés en utilisant une méthode d’éléments fins. Les résultats de l’analyse par éléments fins sont comparés à ceux obtenus dans une étude expérimentale par Perry et al. Cette comparaison montre que les valeurs du champ de déplacement et l’augmentation de ténacité pendant la propagation d’une fissure stable, prédites par l’analyse par éléments fins, sont très semblables à ceux obtenus dans l’étude expérimentale. De plus, le présent modèle est capable de fournir une information détaillée telle que la répartition de la zircone transformée dans le sillage de la fissure.


1. INTRODUCTION

Stress induced phase transformation of zirconia, in ceramic materials, has been found to improve the fracture toughness of such materials [1, 2]. Tetragonal-phase zirconia, which is contained as second phase particles in certain ceramic materials such as zirconia toughened alumina (ZTA) and partially stabilized zirconia (PSZ), undergoes phase transformation to monoclinic structure due to an applied stress. This stress-induced phase transformation results in nonlinear constitutive behavior of the material [3–5]. The phase transformation is associated with 4–6% of volumetric strain, and about 16% of shear, when the particle is free from the constraint of surrounding material [2]. When a macroscopic crack is present in the material, the high stress field around the crack tip induces the zirconia phase transformation, resulting in a significant modification of the linear elastic crack-tip stress field. However, the zone of zirconia
Phase transformation is generally very small compared to the dimension of the structure [6, 7], and is well embedded in the zone of the linear elastic stress field. The stress field outside the transformed zone is almost unaffected by the presence of the transformation zone. Inside the transformation zone, fully and partially transformed zones are both considered to exist [3]. In the fully transformed zone, all the transformable zirconia particles are transformed, and in the partially transformed zone, only a portion of the transformable zirconia particles are transformed. The fully transformed zone is embedded in the partially transformed zone. In the fully transformed zone, the material is considered to behave linearly [3]. The material exhibits a nonlinear constitutive behavior in the partially transformed zone. Thus, if the fully transformed zone exists around the crack tip, the stress immediately near the crack tip has a $1/\sqrt{r}$ type singularity, and is characterized by the crack tip stress intensity factor $K_{ip}$. The stress field outside the transformed zone is characterized by the far field stress intensity factor $K_{fp}$. The stress intensity at the crack tip is reduced under certain conditions, as discussed in a later section. The difference between $K_{ip}$ and $K_{fp}$ is considered to represent the toughness enhancement due to the phase transformation [3, 4].

In order to predict the toughness enhancement, the stress intensity at the crack tip needs to be analyzed.

In this paper, an analysis of the toughness enhancement due to the transformation is presented. The analysis is carried out in a continuum sense, using a nonlinear finite element method. A constitutive model is developed, based on a micromechanics approach. The material is considered to be a two-phase composite material, composed of a matrix and of second phase particles. The second phase particles represent the tetragonal zirconia particles, which transform to a monoclinic structure under an applied stress. The resulting material response exhibits a nonlinear deformation, which is analogous to the plastic behavior of metallic materials. The solid of our interest is designated as transformation plasticity solid (TPS) in this paper. Using a self-consistent approach along with the image strain method, macroscopic and microscopic behaviors of the material are considered. The constitutive model is implemented in a nonlinear finite element code [8]. Problems of stationary and stably propagating cracks are analyzed, and the toughness enhancement in magnesia partially stabilized zirconia (Mg-PSZ) is estimated. A uniaxial stress–strain curve of Marshall [5] is used to determine the behavior of the phase transformation of tetragonal zirconia in Mg-PSZ. By the use of the present constitutive model, the microscopic behavior of the material is revealed. From the results of the analysis of a stably propagating crack, a toughness enhancement of about 40% at the steady state is predicted. Some detailed information about transformation toughening, such as the height of transformed zone, the distribution of the transformed zirconia, transient behavior from the initiation to the steady state, and displacements, is determined numerically. These numerical results are compared with those of a moire inferommetry experiment [9]. Trends in the displacement fields match each other. The height of the wake zone behind the crack tip is predicted from both the experimental and computational results.

### 2. Constitutive Equation for the Transformation Plasticity Solid

In this section, a rate (incremental) type of constitutive equation is developed for the transforming solid. A self consistent method is used to develop the constitutive model, considering three different material constituents; the matrix, and the transformed and the untransformed second phase particles, as shown in Fig. 1. The matrix and the untransformed zirconia particles are considered to have identical properties in the present work. However, for the sake of generality in the ensuing discussions, the matrix and the untransformed tetragonal zirconia particles are treated as different materials.

The phase transformation of tetragonal zirconia is caused by the applied stress. In the present constitutive modeling, the amount of second phase material that is transformed, is assumed to be related to the level of stress in the untransformed tetragonal zirconia. For simplicity in developing the constitutive model, the tetragonal zirconia particles are assumed to be spherical in shape. Although it has been reported that tetragonal zirconia particles in Mg–PSZ are often oval in shape [10], the shape effect may be
small as reported in Wu [11] and in Ramakrishnan et al. [12].

In order to derive a constitutive equation at the macroscopic level, an image strain method along with the self-consistent method [13] is employed. The interaction between a single transformed zirconia particle and the surrounding homogenized material is first discussed. The discussion is initiated without imposing restrictions on the elastic properties of the particle and of the surrounding homogenized material. The surrounding material is assumed to be infinite in space, and to have a uniform initial strain of ε^T_jj. The stress σ_jj and strain ε_jj in the infinite homogenized medium, in the absence of the transformed particle, are assumed to be uniform. The stress σ_jj in the homogenized infinite material can be shown to be

\[ \sigma_{jj} = E_{ijk} (\varepsilon_{kk} - \varepsilon_{ij}^0) \]  

where \( E_{ijk} \) represent the Hooke’s elastic constants of the infinite homogenized medium.

When the detailed structure of a homogenized medium, with a transformed zirconia embedded in it, is modeled, equation (1) still represents the stress-strain relationship of the homogenized medium at infinity. In order to discuss the stress-strain relationship in the transformed zirconia embedded in the infinite homogenized medium, we denote the deviation of the stress and of the strain in the particle, from those of the homogenized medium at infinity, as \( \sigma_{jj}^T \) and \( \varepsilon_{jj}^T \) respectively. These are called the perturbations of stress and strain in the transformed zirconia particle. The transformed zirconia particle is assumed to have a transformation strain \( \varepsilon_{jj}^T \). Thus, by letting the elastic compliance tensor of the transformed zirconia be \( E_{ijk}^T \), the stress \( \sigma_{jj}^T \) and strain \( \varepsilon_{jj}^T \) in the transformed zirconia particle can be expressed as

\[ \sigma_{jj}^T = E_{ijk}^T (\varepsilon_{kk} - \varepsilon_{ij}^0). \]  

In order to consider the interaction between the transformed particles and the surrounding material, the concept of Eshelby’s tensor [14] is used. Eshelby’s tensor can be explained as follows.

When an ellipsoidal inhomogeneity subject to a uniform initial strain \( \varepsilon_{jj}^T \) is embedded in an infinite elastic medium, the strain \( \varepsilon_{jj} \) inside the inhomogeneity is uniform. At this point, the elastic properties of the inhomogeneity are taken to be identical to those of the infinite medium \( E_{ijk}^T \). The strain \( \varepsilon_{jj} \) can be represented by using Eshelby’s tensor \( S_{ijk} \), as

\[ \varepsilon_{jj} = S_{ijk} \varepsilon_{kk}^T. \]  
The stress in the inhomogeneity, \( \sigma_{jj} \), is expressed by

\[ \sigma_{jj} = E_{ijk} (\varepsilon_{kk} - \varepsilon_{ij}^0). \]

When the infinite medium is subjected to stress \( \sigma_{jj}^T \) at infinity, the stress at infinity and in the inhomogeneity are written, respectively, as

\[ \sigma_{jj}^T = E_{ijk}^T (\varepsilon_{kk}^T - \varepsilon_{ij}^0) \quad \text{(at infinity)} \]

\[ \sigma_{jj} = E_{ijk} (\varepsilon_{kk} - \varepsilon_{ij}^0 + \varepsilon_{kk}^T - \varepsilon_{ij}^T) \quad \text{(in the homogeneity)} \]

\[ \varepsilon_{ij} = S_{ijk} \varepsilon_{kk}^T \]

where, \( \varepsilon_{ij}^T \) is elastic strain due to the applied stress \( \sigma_{jj}^T \).

In the present discussion of the interaction between the transformed zirconia particle and the infinite elastic medium, Eshelby’s tensor takes an important role. In order to make use of Eshelby’s tensor, it is necessary to introduce the concept of an image strain method, wherein the difference in elastic properties between the transformed particle and the surrounding matrix, and the existence of the initial (transformation) strains in the particle and in the surrounding medium, are accounted for by a fictitious image strain \( \varepsilon_{ij}^m \). The stress inside the transformed particle is expressed, using the elastic compliance tensor \( E_{ijk} \) of the surrounding medium and the image strain \( \varepsilon_{ij}^m \), as

\[ \sigma_{jj} = E_{ijk} (\varepsilon_{kk}^T - \varepsilon_{ij}^0 + \varepsilon_{kk}^m - \varepsilon_{ij}^m - \varepsilon_{ij}^T). \]  

Here, it is considered that the elastic part of the strain in the infinite medium is \( \varepsilon_{ij} - \varepsilon_{ij}^m \). In equation (4) the perturbation of strain \( \varepsilon_{ij}^T \) in the transformed particle can be considered to be caused by the initial strains \( \varepsilon_{ij}^0 \) and \( \varepsilon_{ij}^m \). Comparing equations (5) and (6), we find that

\[ \varepsilon_{ij}^m = S_{ijk} (\varepsilon_{kk}^m + \varepsilon_{ij}^m) \]

by letting \( \varepsilon_{ij}^T = \varepsilon_{ij} - \varepsilon_{ij}^m \). \( \varepsilon_{ij} = \varepsilon_{ij}^m \), \( \varepsilon_{ij}^m = \varepsilon_{ij}^T \), and \( \varepsilon_{ij}^T = \varepsilon_{ij}^T + \varepsilon_{ij}^m \).

In the present constitutive modeling for partially stabilized zirconia, we are interested in only the dilatational behavior of the material. The elastic properties of the material are assumed to be homogeneous. The long range effect of the shear transformation strain can be considered to be small, because of the kinking and twinning taking place inside the transformed zirconia particles [15], and due to the randomness of the distribution of particles. We consider that only the dilatational behavior is affected by the stress-induced phase transformation at macroscopic level. The distortional components in the transformation strain are neglected in the present work. Therefore, the resulting macroscopic constitutive response is dilatationally nonlinear and distortsionally linear. However, it is noted that a constitutive model, that includes the effects of distortional stress and of deviatoric transformation strain, can be found in the literature [6, 7]. In [6, 7], the shear stress in the transformed particle is assumed to be free from shear stress. This assumption maximizes the effect of the shear transformation strain; this
may be an overestimation. In the present work, the shear transformation strain is neglected. The elastic properties of the material are assumed to be homogeneous.

As a special case of the above discussion on the interactions between the particle and the matrix, only the dilatational behavior is discussed. The hydrostatic tensile stress in the transformed zirconia particle can be written as

\[ \frac{1}{3}(\sigma_{sk} + \sigma_{sk}') = K(\varepsilon_{sk} + \varepsilon_{sk}' - \varepsilon_{sk}^I) \]  

where \( K \) is the bulk modulus of the material.

Using the image strain method, the hydrostatic tensile stress can also be expressed by

\[ \frac{1}{3}(\sigma_{sk} + \sigma_{sk}') = K(\varepsilon_{sk} - \varepsilon_{sk}' + \varepsilon_{sk}' - \varepsilon_{sk}^I) \]  

and

\[ \varepsilon_{sk}^I = \frac{1}{2}S_{ijkl}(\varepsilon_{sk} + \varepsilon_{sk}') \]

\[ \frac{1}{2}S_{ijkl} = \frac{1 + \nu}{1 - \nu} \] (\( \nu \) : Poisson’s ratio) 

while the hydrostatic tensile stress \( \frac{1}{3}\sigma_{sk} \) in the surrounding homogenized medium at infinity is

\[ \frac{1}{3}\sigma_{sk} = K(\varepsilon_{sk} - \varepsilon_{sk}^I). \]  

Now we introduce the concept of self-consistency to the above discussion on the interaction between the transformed particle and the infinite surrounding medium. As mentioned earlier, the material of our interest has three different constituents; the matrix, and the transformed and untransformed particles. The stress \( \frac{1}{3}\sigma_{sk} \) and the strain \( \varepsilon_{sk} \) of the infinite homogenized medium at infinity represent the macroscopic effective stress and the macroscopic effective strain, respectively. The initial strain \( \varepsilon_{sk}^I \) of the infinite homogenized medium represents the macroscopic effective transformation strain of the homogenized material, that is caused by the transformation of particles with the transformation strain \( \varepsilon_{sk} \). Thus, the discussion on the interaction between a transformed particle and the infinite surrounding medium can be regarded as a first order approximation of the mechanical interaction between the particle and the rest of the material.

From equations (8) and (9), we find

\[ \varepsilon_{sk}^I = -\varepsilon_{sk}^I. \]  

From equations (9), (10) and (11), the dilatational strain of the transformed zirconia particle in terms of the macroscopic effective strain, macroscopic effective transformation strain, and the transformation strain of zirconia, can be shown to be

\[ \varepsilon_{sk} + \varepsilon_{sk}' = \varepsilon_{sk} + \frac{1}{3}S_{ijkl}(\varepsilon_{sk} + \varepsilon_{sk}'). \]  

For an untransformed particle, the transformation strain \( \varepsilon_{sk}^I \) is set to be zero. The strain in untransformed particle \( \varepsilon_{sk} + \varepsilon_{sk}' \) is

\[ \varepsilon_{sk} + \varepsilon_{sk}' = \varepsilon_{sk} - \frac{1}{3}S_{ijkl}\varepsilon_{sk}^I. \]  

For Mg–PSZ, the matrix and the untransformed tetragonal zirconia are identical. The stress and strain, which are derived for the untransformed zirconia, represent those for the matrix also. The effective strain \( \varepsilon_{sk} \) and the effective stress \( \frac{1}{3}\sigma_{sk} \) can be determined as the averages of those in all the material constituents. Upon denoting the volume fraction of the transformed zirconia to be \( \chi_T \), the effective stress and strain can be shown to be

\[ \varepsilon_{sk} = (1 - \chi_T)(\varepsilon_{sk} + \varepsilon_{sk}') + \chi_T(\varepsilon_{sk} + \varepsilon_{sk}^I) \]  

\[ \frac{1}{3}\sigma_{sk} = (1 - \chi_T)(\frac{1}{3}(\varepsilon_{sk} + \varepsilon_{sk}')) + \chi_T(\frac{1}{3}(\varepsilon_{sk} + \varepsilon_{sk}^I)) \]  

where \( \frac{1}{3}(\sigma_{sk} + \sigma_{sk}') \) is the hydrostatic tensile stress in the untransformed tetragonal zirconia particles and in the matrix.

From equation (15), we can obtain

\[ 0 = (1 - \chi_T)\varepsilon_{sk}' + \chi_T\varepsilon_{sk}^I \]

and

\[ \varepsilon_{sk}' = C_T\varepsilon_{sk} \]  

Equation (17) has been used in [3, 18, 19]. However the detailed analysis for the particle–global interaction is given here, in order to reveal the behavior of each one of the material constituents. The strain in the transformed zirconia particle and that in the untransformed zirconia particle are shown to be

\[ \varepsilon_{sk} + \varepsilon_{sk}' = \varepsilon_{sk} - \frac{1}{3}S_{ijkl}C_T\varepsilon_{sk}^I \]

\[ \varepsilon_{sk} + \varepsilon_{sk}' = \varepsilon_{sk} + \frac{1}{3}S_{ijkl}(1 - \chi_T)\varepsilon_{sk}^I. \]  

As discussed earlier, the constitutive equation that is sought in this study is of a rate form, and a relationship between the stress in the untransformed second phase particle and the volume fraction of the transformed zirconia particles is assumed to exist (see Fig. 2). The slope of the curve in Fig. 2 gives the rate of the phase transformation.

\[ C_T = \frac{h}{\frac{1}{3}(\varepsilon_{sk} + \varepsilon_{sk}')} \cdots \frac{1}{3}(\sigma_{sk} + \sigma_{sk}') > 0 \]

\[ C_T = 0 \cdots \frac{1}{3}(\sigma_{sk} + \sigma_{sk}') < 0 \]  

Fig. 2. The volume fraction of transformed zirconia as a function of the hydrostatic tensile stress inside untransformed zirconia particles.
and
\[ h = h[(\delta_{kk} + \sigma_{kk}^{tr})], \text{ etc.} \]  

(21)

where (’) denotes the time derivative. \( h \) is the slope of the curve depicted in Fig. 2.

Equations (20) and (21) form the basis of the constitutive equation developed in this study. The effective stress, which is the stress in the untransformed tetragonal zirconia particle, is \( (\delta_{kk} + \sigma_{kk}^{tr}) \) in the present study for the transformation plasticity. This is very analogous to the equivalent stress \( \sqrt{\sigma_{ij} \sigma_{ij}} \) in the case of metal plasticity. When this effective stress is increasing, the material response is nonlinear (loading), and when the effective stress is decreasing, the material response is linear (unloading). As in the case of metal plasticity, a rate form description is adequate in the description of transformation plasticity also, as well as its loading-unloading behavior.

From equation (18), the rate of the stress in the untransformed tetragonal zirconia can be expressed by
\[
\frac{1}{2}(\dot{\delta}_{kk} + \sigma_{kk}^{tr}) = K(\dot{\epsilon}_{kk} + \epsilon_{kk}^{tr}) = K(\dot{\epsilon}_{kk} - \frac{1}{2}S_{kk}^{ij} \dot{\epsilon}_{kk}).
\]

(22)

Also from equation (17),
\[
\dot{\epsilon}_{kk} = C_{T} \dot{\epsilon}_{kk}.
\]

(23)

From equations (20), (22) and (23), a formula for the rate of hydrostatic tensile stress in untransformed tetragonal zirconia can be derived as
\[
\frac{1}{2}(\dot{\delta}_{kk} + \sigma_{kk}^{tr}) = \frac{K\dot{\epsilon}_{kk}}{1 + \frac{1}{2}K\dot{\sigma}_{ij} \dot{\epsilon}_{kk}}.
\]

(24)

Using equations (20), (23) and (24), we obtain an expression for \( \dot{\epsilon}_{kk}^{T} \)
\[
\dot{\epsilon}_{kk}^{T} = \frac{\epsilon_{mn}^{T} hK\dot{\epsilon}_{kk}}{1 + \frac{1}{2}K\dot{\sigma}_{ij} \dot{\epsilon}_{kk}}.
\]

(25)

Therefore, the rate form constitutive equation can be written as follows
\[
\dot{\delta}_{ij} = \dot{\epsilon}_{ij} K \left( 1 - \frac{\epsilon_{mn}^{T} hK}{1 + \frac{1}{2}K\dot{\sigma}_{ij} \dot{\epsilon}_{kk}} \right) \dot{\epsilon}_{kk} + 2\mu \dot{\epsilon}_{ij}^{T},
\]

(26)

when \( \frac{1}{2}(\dot{\delta}_{kk} - \dot{\sigma}_{kk}^{tr}) \geq 0 \) and
\[
\dot{\delta}_{ij} = \dot{\epsilon}_{ij} K\dot{\epsilon}_{kk} + 2\mu \dot{\epsilon}_{ij}^{T},
\]

(27)

when \( \frac{1}{2}(\dot{\delta}_{kk} - \dot{\sigma}_{kk}^{tr}) < 0 \), where \( \dot{\epsilon}_{ij} \) is the rate of effective deviatoric strain. This constitutive model will be employed to analyze an evaluation of toughness enhancement of Mg-PSZ during a stable crack propagation.

### 3. TOUGHENING MECHANISM

In this section, the enhancement of the fracture toughness in mode I loading case (opening mode) is discussed. The response of the material is linear, after all the transformable zirconia particles transform their phase to monoclinic structure. The material is assumed to behave linearly around the crack tip, and the stresses have a \( 1/\sqrt{r} \) type singularity at the crack tip. The severity of the stress condition around the crack tip can be characterized by the stress intensity factor \( K_{I} \). Also, as reported in [7], the size of the transformed zone around the crack tip is of the order of 10 \( \mu \)m and is generally found to be much smaller than the size of the structure. Thus we can also introduce the concept of small scale yielding of metal plasticity to the transformation plasticity case; that is, the nonlinear deformation zone (transformation zone) is small, and is well embedded in the \( 1/\sqrt{r} \) singular stress field of the linear elasticity. The stress intensity at the crack tip is characterized by the crack tip stress intensity factor \( K_{I}^{tr} \) and that outside the transformed zone the stress field is governed by the far-field stress intensity factor \( K_{I}^{far} \) [3, 4]. The toughness increment is shown by the difference between \( K_{I}^{tr} \) and \( K_{I}^{far} \). It is assumed here that the critical value of the crack tip stress intensity factor \( K_{I}^{tr} \) is a material property, and is unchanged by the transformation of zirconia particles.

The path independent integrals \( J \) and \( T^{*} \) are employed to evaluate the enhancement of the fracture toughness using the finite element analysis. Both the \( J \) integral [20] and the \( T^{*} \) [21] integral have their basis in the energy release per unit crack extension. The \( J \) integral is limited to the case of self-similar crack extension in linear or nonlinear elastic solids under static loading, whereas the \( T^{*} \) integral can be applied to the case of general nonlinear solids under dynamic loading [2]. The \( J \) and \( T^{*} \) integrals are defined by (for quasi static case)
\[
J = \int_{\Gamma} (Wn_{1} - n_{i}\sigma_{ij} u_{ij}) \, d\Gamma
\]

(28)

\[
T^{*} = \int_{\Gamma} (Wn_{1} - n_{i}\sigma_{ij} u_{ij}) \, d\Gamma
\]

(29)

where \( W = \int_{\Gamma} n_{i} u_{ij} d\Omega \) and \( (.)_{i} \) represents spatial derivative. The integral contour \( \Gamma \) and region \( \Omega - \Omega^{*} \) are shown in Fig. 3. Since these two integrals compute the energy release rate, one can show the relations to the crack tip stress intensity factor and the far field stress intensity factor to be
\[
J = \frac{1 - v^{2}}{E} (K_{I}^{tr})^{2}
\]

(30)

\[
T^{*} = \frac{1 - v^{2}}{E} (K_{I}^{far})^{2}
\]

(31)
Fig. 3. Integral path and area for $J$ and $T^*$ integral.

Equations (30) and (31) are valid only for the mode I crack case under plane strain condition and the integral path $\Gamma$ is taken from the crack tip transformed zone. For the mixed mode cases, other terms of the mode II and the mode III stress intensity factors appear in the right hand side of equations (30) and (31). From these path independent integrals, we can calculate the stress intensity factors. The crack tip stress intensity factor and the far field stress intensity factor are found, from equations (28)-(31), to have the following relationship

$$\frac{1 - v^2}{E} (K_I^{op})^2 = \frac{1 - v^2}{E} (K_I^{op})^2 - \int_{\Gamma - \alpha} (W_{ij} - \tau_{ij}) \, d\Omega$$

(32)

The fracture toughness enhancement can be estimated by evaluating the volume integral term in equation (32).

For the stationary crack case, the transformed zone is created ahead of the crack tip and no material particle undergoes the unloading path (see Fig. 4). It can be shown that the volume integral term in equation (32) is equal to zero. Therefore, no toughness enhancement is seen in this case (i.e. the crack tip and the far field stress intensity factors are equal to each other). In the case of stable crack propagation, the transformed zone is left behind the crack tip where the material undergoes unloading and the volume integral term in equation (32) is not equal to zero. The fracture toughness enhancement is seen in this case. Equation (32) can be simplified for a dilatational transformation plasticity model as

$$\frac{1 - v^2}{E} (K_I^{op})^2 = \frac{1 - v^2}{E} (K_I^{op})^2 - \int_{\Gamma - \alpha} \left( \frac{\partial}{\partial x_i} \left( \int_0^{\alpha} \frac{1}{2} \sigma_{ij} \, d\epsilon_{ij} \right) - \frac{1}{2} \sigma_{ij} \epsilon_{ij,1} \right) \, d\Omega$$

(33)

4. EVALUATION OF TOUGHNESS ENHANCEMENT OF Mg-PSZ

4.1. Determination of material constants

The present dilatational transformation plasticity model is applied to Mg-PSZ. The elastic properties are available in [22]. The uniaxial stress–strain curve [5†] is used to determine the transformation behavior. Stationary and stably propagating cracks are analyzed using a finite element method, in which the present constitutive model is implemented.

The uniaxial stress–strain curve [5†], which is shown in Fig. 5, can be empirically expressed, as

$${\sigma} = E\epsilon$$

$$\sigma < \sigma_Y (\text{MPa})$$

$$\sigma = E(\epsilon - \epsilon_0)^n - \sigma_0 (\text{MPa}) \quad \sigma \geq \sigma_Y (\text{MPa})$$

(34)

Fig. 4. A typical dilatational stress–strain hysteresis of transformation plasticity solid.

In the limiting case of a semi-infinite crack, equation (33) can be further simplified and it becomes identical to the formula given in Budiansky et al. [3]. It is then considered that the far field stress intensity factor $K_I^{op}$ gradually approaches this asymptotic value during the stable crack growth.

†MS-grade Mg-PSZ, Nilcra Ceramics (U.S.A.) Inc.

Fig. 5. Uniaxial stress–strain curve for Mg–PSZ by Marshall [5].
Where

\[ E = 208,000 \text{ (MPa)} \]
\[ \sigma_Y = 280 \text{ (MPa)} \]
\[ \epsilon_0 = 0.99717 \times 10^{-3} \]
\[ \sigma_0 = 0.2071 \times 10^6 \text{ (Pa)} \]
\[ N = 3.5 \times 10^{-4}. \]

From this expression, the relationship, as shown in Fig. 6, between the volume fraction of transformed zirconia and the stress in untransformed zirconia particles can be obtained. The curve shown in Fig. 6 was obtained as follows. Assuming the material to be distortionally linear and the state of stress to be uniaxial (\( \sigma_{kk} = \sigma \)), the instantaneous bulk modulus \( \tilde{K} \) can be derived as

\[ \tilde{K} = \frac{\tilde{E}_\mu}{9\mu - 3\tilde{E}} \]  

(35)

where \( \tilde{E} \) is the slope of the curve given in Fig. 5 and \( \mu \) is the shear modulus.

\[ \tilde{E} = E^{1/N}N(\sigma - \sigma_0)^{N-1}/N. \]  

(36)

In the constitutive equation (26), the instantaneous bulk modulus \( \tilde{K} \) is expressed by

\[ \tilde{K} = K \left( 1 - \frac{\tilde{E} \mu hK}{1 + \frac{1}{3} KhS_{\text{hy}} \epsilon_{kk}} \right). \]  

(37)

From equations (35) and (37), \( h \) can be determined as

\[ h = \frac{E \epsilon_{kk}}{9(1 - v)(E - \tilde{E})} \left( 2E - (1 + v)\tilde{E} \right). \]  

(38)

The volumetric component of the rate of effective strain \( \dot{\epsilon}_{kk} \) can be expressed by

\[ \dot{\epsilon}_{kk} = \frac{1}{3} \dot{\sigma}_{kk}/\tilde{K} = \frac{\dot{\sigma}}{\tilde{K}}. \]  

(39)

Using the expression for \( \tilde{E} \) (36) in (35), and integrating both sides of equation (39) with respect to time, the volumetric component of the rate of effective strain can be determined as

\[ \dot{\epsilon}_{kk} = \frac{3}{(1 - 2v)} \frac{(\sigma - \sigma_0)}{\sigma_Y}. \]  

(40)

From equations (24) and (39), we have

\[ \frac{1}{3} (\dot{\sigma}_{kk} + \dot{\sigma}_{kk}^T) = \frac{K}{1 + \frac{1}{3} KhS_{\text{hy}} \epsilon_{kk}} \left( \frac{\dot{\sigma}}{\tilde{K}} \right). \]  

(41)

Substituting the expressions for \( h \) (38) and for \( \tilde{K} \) (35) in equation (41), and integrating both sides of equation (41), the hydrostatic tensile stress in untransformed t-zirconia particle can be derived as

\[ \frac{1}{3} (\sigma_{kk} + \sigma_{kk}^T) = \frac{1}{2} \left[ \frac{2E}{(1 - v)} \left( \frac{(\sigma - \sigma_0)^{1/N}}{E} \right) \right. \]
\[ - \left. \left( \frac{\sigma_Y - \sigma_0}{E} \right)^{1/N} \right] - (1 + v)(\sigma - \sigma_Y) + \frac{1}{2} \sigma_Y. \]  

(42)

Likewise, an expression for the volume fraction of transformed zirconia can be derived, and is shown to be

\[ C_T = \frac{3}{\epsilon_{kk}} \left\{ \left( \frac{\sigma - \sigma_0}{E} \right)^{1/N} \right. \]
\[ \left. - \left( \frac{\sigma_Y - \sigma_0}{E} \right)^{1/N} \right\} - (1 + v)(\sigma - \sigma_Y) / \frac{\sigma_0 - \sigma_Y}{E}. \]  

(43)

Therefore, the relationship between the hydrostatic tensile stress of untransformed zirconia and the volume fraction of transformed zirconia can be determined from (43) and (42), as a parametric function.
of $\sigma$, as shown in Fig. 6. The effective volumetric strain–hydrostatic tensile strain curve can be determined by letting $\sigma$ be $\delta_{kk}$ in (40), and is shown in Fig. 7. Also, by letting $\sigma$ be $\delta_{kk}$ in expressions (38), (40), (42) and (43), $\varepsilon_{kk}$, $\frac{1}{2}(\delta_{ik} + \delta_{ik})$ and $C_T$ can be shown, in terms of effective hydrostatic tensile stress $\frac{1}{3}\delta_{kk}$. The present constitutive model is useful for understanding the micro–macro interaction in the deformation mechanisms. For example, a curve for the relationship between effective hydrostatic tensile stress and hydrostatic tensile stress in matrix and untransformed zirconia is shown in Fig. 8. It is clear that the stress in matrix and untransformed zirconia is much more severe compared to the effective stress. Such behavior can only be revealed by consideration of the macro–micro interactions of deformation mechanisms, which have been carried out in the present constitutive modelling.

Although the uniaxial stress–strain curve given by Marshall [5] terminates without the linear portion of full transformation, it is assumed in the present analysis that the linear portion of full transformation exists from the terminal point in Fig. 4.$^t$ Poisson’s ratio $\nu$ is assumed to be 0.23, according to [22]. The transformation strain $\varepsilon_{kk}^T$ is taken to be 0.04.

4.2. Stationary crack analysis

The analysis of stationary crack is presented in this section. The present transformation plasticity constitutive equation is implemented in a nonlinear finite element code [8]. Four-noded isoparametric elements with $2 \times 2$ Gauss quadrature are employed. The analysis is carried out under plane strain condition. In order to ensure the existence of a stress field outside of the transformed zone, that is dominated by the far field stress intensity factor, the $K^\text{tr}$ field is imposed by the displacement boundary condition. A semi-circular zone, as shown in Fig. 9, is analyzed with the given displacement boundary condition on its circular arc. The given displacement boundary condition can be written as

$$u_i = \frac{K_{1}^\text{tr}}{2\mu} \sqrt{\frac{r}{2\pi}} f_i(\theta)$$

where

$$f_1(\theta) = \cos \frac{\theta}{2} \left( 2 - 4\nu + 2\sin^2\frac{\theta}{2} \right)$$

$$f_2(\theta) = \sin \frac{\theta}{2} \left( 2 - 4\nu - 2\cos^2\frac{\theta}{2} \right).$$

This is the asymptotic solution for displacements under the mode I loading condition with the stress intensity factor $K_{1}^\text{tr}$. The finite element mesh discretization is also shown in Fig. 9. The total number

$^t$The stress–strain curve given in Fig. 5 terminates at the point A', but in the present analysis, we assume a linear relationship in the hydrostatic tensile stress–dilatational strain curve from the corresponding point A, as shown in Fig. 7.
OKADA et al.: TOUGHENING OF MAGNESIA PARTIALLY STABILIZED ZIRCONIA

1429

I I

~ / Elastic solution

Mg-Psz

0 1 2 3 4
Distance from crack tip: r/\bar{r} (x 10^6)

1

\bar{r} = \frac{1}{2\pi} \left( \frac{K_1}{E} \right)^2

Fig. 11. Variation of stress \( \sigma_{yy} \) ahead the crack tip in Mg-PSZ for stationary crack case.

of elements and nodes are 960 and 1025. The size of the transformed zone is set to be smaller than 1–2% of the radius of the semi-circular region, so that the small scale yielding condition is appropriately represented.

The transformed zone shape is shown in Fig. 10. It is seen that the fully transformed zone is very small compared to the size of the partially transformed zone. The stress ahead of the crack tip is also depicted in Fig. 11; it gradually decreases towards the crack tip. In Fig. 12, the stress ahead the crack tip normalized by that of linear elasticity solution is shown. If the fully transformed zone does not exist around the crack tip, the stress intensity at the crack tip is reduced.

4.3. Stable crack propagation analysis

For stable crack propagation analysis, a problem of semi-circular region, to which the far field \( K_1 \) dominant field is imposed, is also chosen. At the boundary of the semi-circular region, the displacement boundary condition, as given by (44), is imposed. The semi-circular region is shown in Fig. 9. The finite element mesh discretization is given in Fig. 13. The crack tip is initially at point (i) in Fig. 13(c), and is move to point (ii), using a nodal release technique. Only one node is released at a time. Associated with the nodal release procedure, the \( T^* \) integral is kept constant. It is noted here that the far field \( K_1 \) governing field, which is imposed by the boundary condition, does not exactly satisfy the \( K_1 \) asymptotic field for the crack tip position during the process of crack propagation, because the crack tip is slightly off from the center of the circular arc of the semi-circular region. However, the offset of the crack tip position is less than 3% of the radius of the circular arc, so that the deviation of the \( K_1 \) asymptotic field, which is imposed by the boundary condition, from that actually imposed for the current crack tip position is negligibly small. We assume that the value of \( K_1 \) in equation (44) represents the far field stress intensity factor \( K_1^{\infty} \). As discussed earlier, the crack tip stress intensity factor \( K_1^{\infty} \) is assumed to be unchanged throughout the process of the crack propagation. \( K_1^{\infty} \) and \( K_1^{\infty} \) are identical at the initiation of crack propagation as mentioned previously. We assume that \( K_1 \) in equation (44) can

\[ \bar{r} = \frac{1}{2\pi} \left( \frac{K_1}{E} \right)^2 \]

Distance from crack tip: r/\bar{r} (x 10^6)

\[ \bar{r} = \frac{1}{2\pi} \left( \frac{K_1}{E} \right)^2 \]

Fig. 12. Variation of stress \( \sigma_{yy} \) ahead the crack tip, normalized by the solution of linear elasticity.

Fig. 13. Finite element mesh discretization for stable crack propagation problem (5640 elements, 5787 nodes).
OKADA et al.: TOUGHENING OF MAGNESIA PARTIALLY STABILIZED ZIRCONIA

Fig. 14. Algorithm for crack tip stress intensity factor $K_{ip}^p$ (and $T^*$ integral) constant crack propagation analysis.

Fig. 15. Toughness enhancement during stable crack propagation (R-curve) of Mg-PSZ, obtained by finite element method.

represent the far field stress intensity factor. Also, the crack tip intensity factor $K_{ip}^p$ can be calculated from $T^*$ integral value as

\[ K_{ip}^p = \frac{E}{\sqrt{1-v^2}} T^*. \tag{45} \]

In the nodal release technique, the external load is chosen in each nodal release step such that the $T^*$ integral remains constant. Since the stress–strain response of the TPS has a loading–unloading hysteresis behavior, the hysteresis of each material element must be captured correctly. An iterative algorithm is employed to find the appropriate external load increment for the given nodal release force. The algorithm is shown in Fig. 14. While the crack tip stress intensity factor $K_{ip}^p$ is kept constant, the far field stress intensity factor is assumed to be identical to $K_i$ in equation (44).

Since $K_{ip}^p$ takes a constant value, which is also equal to the value of far field stress intensity factor at the initiation of crack propagation, toughness enhancement during the stable crack propagation can be defined as

\[ \text{toughness enhancement} = \frac{K_{ip}^p}{K_i^\text{far}} - 1. \tag{46} \]

In the current analysis, the stress intensity factor at the initiation $K_{ip}^p$ is assumed to be 4.5 (MPa m$^{1/2}$), which is a value obtained in the experimental study of Perry et al. [9].

The toughness enhancement during the stable crack growth with a constant crack tip stress intensity factor is shown in Fig. 15. A toughness enhancement of 40% is seen in the steady state. In the experimental study of Perry et al. [9], nearly the same order of the toughness enhancement in the steady state is reported and their R-curve is shown in Fig. 16. Although, there is a small discrepancy between the result of the present analysis and that of the experimental study, it can be said that the transformation plasticity is the major source of the toughness enhancement in the case of the partially stabilized zirconia. A common trend, seen in Figs 15 and 16, is that the most of fracture toughness enhancement effect is obtained within a very small length of crack propagation. The growth of the partially transformed zone is depicted in Fig. 17. After the initiation, the transformed zone height rapidly increases, approaching the steady state transformed zone height. From Figs 15 and 17, it is seen that while the far field stress intensity factor is

Fig. 16. R-curve obtained in the experimental study of Perry et al. [9].

\[ 10^6 \tau = 0.053 \, (\text{mm}) \]

\[ \tau = \frac{1}{2K_i^\text{far}} (K_i^\text{initiation} / E)^2 \]

Fig. 17. The growth of partially transformed zone during stable crack propagation in Mg-PSZ, estimated by the finite element analysis.

\[ \Delta a = 0.0 \quad \Delta a = 0.35 \quad \Delta a = 0.70 \quad \Delta a = 1.05 \quad \Delta a = 1.40 \, (\text{mm}) \]

\[ \Delta a = 0.35 \quad \Delta a = 1.05 \quad \Delta a = 1.40 \, (\text{mm}) \]

\[ \Delta a = 0.35 \quad \Delta a = 1.05 \quad \Delta a = 1.40 \, (\text{mm}) \]

\[ \Delta a = 0.35 \quad \Delta a = 1.05 \quad \Delta a = 1.40 \, (\text{mm}) \]
initial crack tip

Crack tip

Fig. 18. Iso-y-displacement curve, obtained from the result of finite element analysis.

increasing, the height of the transformation also increases. The transformed zone height is estimated to be 0.16 mm at the initiation of the crack propagation. The height of the transformed zone in steady state is approximately twice that at the initiation, as seen in Fig. 17; the steady state zone height is estimated to be 0.33 mm.

The iso-y-displacement contour generated from the result of the finite element analysis is shown in Fig. 18; it can be compared to the experimental observation of the moire interferometry [9] which is shown in Fig. 19, which also shows iso-y-displacement curves. Near the free surface behind the crack tip, the iso-y-displacement contour shifts towards the opposite direction of the crack propagation; this is the effect of the irreversible strain produced by the zirconia phase transformation. In Fig. 19, the distance from the crack plane at which the iso-y-displacement curve starts shifting is estimated to be 0.16 mm using the finite element analysis; according to the experimental observation [9], it is 0.11 mm. The patterns of iso-y-displacement curves from the finite element analysis agree with those of the experiment of Perry et al. [9] excellently.

5. DISCUSSION AND CONCLUSIONS

In the application of the present transformation plasticity model to partially stabilized zirconia (Mg-PSZ), the total toughness enhancement in the experimental study of Perry et al. [9] was found to be in agreement with the results of the present study. The transformation zone height is estimated to be 330 μm, but the zone height presented in the other investigations [6, 7] is 0.2-70 μm. The discrepancy between the values reported in [6, 7] and that estimated in the present investigation seems to be large. This could possibly be due to the difference in material properties and crack geometry, and may be even due to the definition of the transformed zone itself. The transformed zone in this study is defined as the region of material in which the volume fraction of the transformed zirconia is not zero. Nevertheless, the results of both the present analysis and the experiment (Perry et al. [9]) are consistent in the deformation patterns observed in the iso-y-displacement curve. Also, in both the cases, most of the toughness enhancement is achieved within a very short length of the crack extension (twice of the height of the initial transformed zone height).

In Fig. 20, the volume fraction of the transformed zirconia is plotted against the distance from the crack plane in the steady state. The curve shows that only 1/3 or 1/4 of the transformed zone contains a considerable amount of the transformed zirconia. A similar result for the volume fraction of the transformed zirconia against the distance from the crack plane is presented by Cox et al. [6]. Recently, Mori et al. [23] also presented a variation of the volume fraction of the transformed zirconia against the distance from the crack plane for Y-PSZ. Both works (Cox et al. [6] and Mori et al. [23]) clearly demonstrate that the variation in the volume fraction of the transformed zirconia is monotonically decreasing from the crack plane. These experimental observations suggest that a similar variation also needs to

Fig. 19. Moire fringe of Perry et al. [9].

Fig. 20. Volume fraction of transformed zirconia in the steady state wake zone, predicted by finite element analysis.
be modelled in an analytical study. The present TPS model is capable of predicting such a variation. The moiré fringe pattern obtained from the present finite element analysis predicts larger wake zone height than the experimental study. One possible explanation is that the plane strain condition is assumed in the finite element analysis. Under the plane strain condition, the hydrostatic tensile stress is certainly larger than that under plane stress condition. The method of two-dimensional idealization for the analysis of transformation toughening is still controversial.

On the other hand, as seen in a recent paper of Dadkhah et al. [24], the displacement field in the wake zone is neither under plane strain nor under plane stress condition. The displacement field is very three-dimensional, because of a surface uplifting due to the dilatational transformation strain on the wake zone, which is also shown in Cox et al. [6]. This surface uplifting can be captured only by three dimensional analysis. The mechanics of fracture in such a case has not been explored fully yet. Although Dadkhah et al. [24] analyzed the surface uplifting in a steady state wake zone, three dimensional effects on the phenomenon of toughness enhancement have not been fully understood. The present constitutive model can be implemented in a three dimensional nonlinear finite element code, and crack problems can be analyzed. In the present paper, the nature of toughening mechanisms has been revealed by two dimensional crack analyses. But, to capture the three dimensional nature of transformation toughening phenomenon, the authors strongly feel a need for a complete three dimensional analysis of the mechanisms of transformation toughening.

Acknowledgement—This work was supported by the Materials Division of the U.S. Army Research Office, with Dr Kailasam R. Iyar as the responsible program official. This support is gratefully acknowledged.

REFERENCES

22. Nilsen (U.S.A.) Inc., Technical data of Nilsen's PSZ.