Modeling of transformation toughening in brittle materials

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Abstract

Results from modeling of transformation toughening in brittle materials using a discrete micromechanical model are presented. The material is represented as a two-dimensional triangular array of nodes connected by elastic springs. Microstructural effects are included by varying the spring parameters for the bulk, grain boundaries, and transforming particles. Using the width of the damage zone and the effective compliance (after the initial creation of the damage zone) as measures of fracture toughness, we find that there is a strong dependence of toughness on the amount, size, and shape of the transforming particles, with the maximum toughness achieved with the higher amounts of larger particles.

1. Introduction

A number of approaches have been taken to improve the fracture toughness of brittle materials. One such approach, called transformation toughening, involves including particles of metastable tetragonal zirconia (ZrO_2) that undergo a martensitic transformation to the larger-volume (\( +4\% \)) monoclinic structure in the stress field near the vicinity of a crack tip [1]. The zirconia particles are stabilized in the tetragonal structure by alloying and by the constraints of the ceramic matrix. High stresses can trigger the irreversible transition to the stable monoclinic structure in a region around the crack tip, referred to as the transformation zone. This approach has been used to improve the fracture toughness of alumina–zirconia composites [2]. Recent work by Petrovic and coworkers [3–5] demonstrated that dispersed particles of stabilized ZrO_2 also increase the fracture toughness of MoSi_2-based materials.

There have been many theoretical studies of transformation toughening that have tried to correlate the increase in toughness with the size and shape of the transformation zone around the crack tip [6]. Generally, these studies have modeled the transformation zone as a linear-elastic continuum, and have considered the case of dilatational transformations triggered by a critical mean stress. Recently, Stump [7] has extended the continuum-mechanics approach to include the effects of a discrete array of particles. This was done by embedding a random distribution of small, discrete, circular inclusions in an elastic matrix surrounding the tip of a semi-infinite crack. These inclusions could undergo a transformation when the stress on them was greater than a set amount. Prior to transformation, the spots and matrix were homogeneous, linear elastic media described by isotropic constants \( E \) and \( v \). Stump considered not only the usual case of purely dilatational transformations triggered by a mean-stress criterion but also the general case with shear transformation stresses and strains. He related the size and shape of the transformation zone as a function of the transformation criteria to the fracture toughness.

One drawback to the continuum mechanics calculations is that it is difficult to include the effects of microstructure on the fracture properties of the material. Additionally, the continuum mechanics results were restricted to the case of the transformation zone around a stationary crack. Experiments [5] show that there is considerable microcracking around the transformed particles. To examine the role of microstructure and microcracking, we have taken another approach, namely a ball-and-spring model [8, 9]. In the next section we shall outline the approach as applied to transformation toughening and describe the role of microstructure on the damage zone in a strained material.

2. Discrete micromechanical model

Extension of the modeling to include the effects of microstructure and microcracking requires a different
approach than that used in the partially discrete micromechanical model developed by Stump [7]. We use a "ball-and-spring" approach, where we treat the system as a two-dimensional triangular lattice of nodes, each of which is connected to its six nearest neighbors by elastic springs. The energy of this system is given by

$$E = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{6} k_i (r_{ij} - r_{ij}^0)^2$$

where $k_i$ is the force constant and $r_{ij}^0$ is the equilibrium length of the spring connecting node $i$ to node $j$. Fracture occurs when the spring length $r_{ij}$ exceeds the breaking strain $r_{ij}^b$. The unstressed topology of the model is shown in Fig. 1. We note that the elastic properties of this system are those of an isotropic solid. While the model can be improved by including three-body (angular) interactions [9], for the present study we restrict the model to two-body interactions.

The microstructure is generated with a Potts model, which has been shown to yield realistic grain-size distributions [10]. The Potts model is similar to an Ising model, except that, instead of having only two possible spin values, many values are allowed. Areas with different spin values correspond to different grains. A typical section of the system is shown in Fig. 2. The line marking the region between grains is a grain boundary. S represents a second-phase particle. The key to the utility of the model is that springs can be assigned different parameters depending on whether they connect nodes within the same grain, nodes in different grains, or nodes connected to second-phase particles. Thus, we can model competing fracture mechanisms.

We assume that all bulk grains are alike and that there is no orientational dependence in the grain-boundary properties. Thus, all bulk springs (within the grains, e.g. the 1–1 interaction in Fig. 2) are defined by the three spring parameters $k_B$, $r_{B}^0$, and $r_{B}^b$. The properties of springs crossing grain boundaries (e.g. 1–2 in Fig. 2) are given by $k_{gb}$, $r_{gb}^0$, and $r_{gb}^b$. Similarly, springs connected to second-phase particles (e.g. S–1 in Fig. 2) have properties $k_S$, $r_{S}^0$, and $r_{S}^b$. Transformation of a second-phase particle is modeled by irreversibly increasing the equilibrium spring length $r_{gb}^b$ to $r_{gb}^{b,T}$ when the mean stress on the second-phase particle exceeds a prescribed critical stress $\sigma_c$. For all the calculations described here, $k_B = k_{gb} = k_S = 1 = r_{B}^0 = r_{gb}^0 = r_{S}^0$. Based on a typical experimental value for ZrO$_2$, we assume that there is a 1% increase in the length of the springs connected to second-phase particles upon transformation, i.e. $r_{gb}^{b,T} = 1.01$. The breaking strain for the bulk bonds is $r_{B}^b = 1.005$ and for the grain boundaries and second-phase particles $r_{gb}^b = r_{S}^b = 1.003$. We note that this choice of breaking strain ensures that there should be a mixture of transgranular and intergranular fracture [8]. Finally, we assume a mean-stress criterion for transformations with a critical stress $\sigma_c = 1.001$. These parameters were obviously not chosen to match the exact properties of MoSi$_2$, but rather to incorporate in an approximate way the basic phenomena associated with transformation toughening.

The calculations proceed as follows. An initial distribution of grain boundaries and second-phase particles is assigned to the system, which is then strained in the $x$ direction (Fig. 1) by a finite amount. The energy of the system is minimized with respect to the positions of the nodes. If the mean stress on any second-phase particles is greater than $\sigma_c$, then we transform the particle with the largest stress and minimize the energy with respect to positions again. We iterate until no more particles transform. We then check to see if any spring has a length greater than its breaking strain. If so, we irreversibly break the spring.
with the largest ratio of $r_{ij}$ to $r_{ij}^b$ and minimize the energy again. We iterate until no more springs break. We then check to see if any particles transform, and so on. Once no more particles transform and no more springs break, the strain is increased and the procedure is repeated. We note that the iterative procedure used here is not unique; other schemes are being investigated.

In Fig. 3(a), we show the basic microstructure of the 100 x 100 lattice of nodes used in all simulations reported here. The black lines are grain boundaries generated by a Potts model and the gray wide line is an initial crack created by breaking some of the springs prior to starting the calculations. The system was then strained in small discrete steps until fracture. Since the breaking strain of the springs is 0.003 for the weakest springs, we chose a strain step of 0.0001, which should provide sufficient resolution. In Fig. 3(b), we show the results for total strain of 0.003. Once again, the broad gray line is the fracture path. We note that since periodic boundaries are used in the simulation, when the crack leaves the left-hand side of the cell, it re-appears on the right. In Fig. 3(c), we show the stress-strain curve for this case. We note that the material behaves completely elastically until a strain of 0.003 and then breaks completely. That the fracture was complete is seen by the flat stress as a function of strain, i.e. the material is being pulled apart with no resistance. Examining the fracture path in Fig. 3(b), we see that there is a mixture of intergranular and transgranular fracture.

In Fig. 4(a), we show the initial condition for a case where we have included 10% (by number) second-phase particles (light gray) placed at random on the same microstructure as used in Fig. 3. Applying a strain to the system results in markedly different behavior from the system with no second-phase particles. In Fig. 4(b), we show that the system is damaged at a strain of 0.0015, half that necessary for failure of the system with no transforming particles. We note that the crack is not continuous and fails to span the system, i.e. the system has not failed. A transformation zone develops in front of the initial crack tip and is accompanied by microcracking around the transforming particles, in agreement with experimental observations [5]. Straining the system further to a net strain of 0.003 yields Fig. 4(c). Note that the microcracks have seemingly coalesced into one, continuous crack. However, the stress–strain curve in Fig. 4(d) does not show a flat response of stress vs. strain as expected if the system had failed, thus indicating that the crack is not continuous across the system. Indeed, the system has not failed up to a total strain of 0.005. The damage was initiated at a strain half that of the material with no second-phase particles, an example, perhaps, of microshielding of the crack tip. If one were to use the critical stress as a measure of toughness, then it would imply that the addition of second-phase particles actually impairs the properties of these materials. However, the fracture zone is broader than with no second-phase particles and the system can be strained to a significantly higher extent without failure, so clearly a

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![Fig. 3](image-url)  
(a) Basic microstructure used in 100 x 100 simulations. The dark lines are grain boundaries and the heavy gray line is an initial crack. Note that we have tilted the figure by 30° to fit better on the page (see Fig. 1). (b) The system at a total strain of 0.003. Note that the crack has moved completely across the sample. Because of the periodic boundary conditions along the x-direction (Fig. 1), the crack moved off the left-hand side of the cell and back in on the right. (c) Stress–strain curve.

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different definition of toughness is necessary. We shall return to this point below.

In Fig. 5(a), we show a system with 20% randomly placed second-phase particles at a strain of 0.0015. The most obvious difference between this case and that with 10% transforming particles (Fig. 4(b)) is that the 20% system has a much broader transformation–damage zone. Once again, the system has clearly not failed at this stress. In Fig. 5(b), we show the same system at a strain of 0.003. The damage zone has broadened, but otherwise the system behaves very similarly to that with 10% particles. The stress–strain curve in Fig. 5(c) indicates that the system has not failed at a strain of 0.005.

We show results with 30% randomly placed second-phase particles at a strain of 0.0012 in Fig. 6(a). Note that a transformation zone (with microcracking) has developed in front of the crack tip. Comparison of the shape of the transformation zone with that found with the partially discretized continuum mechanics [7] shows clear differences, largely associated with microcracking around the transforming particles, which is not included in the continuum mechanics calculations. In Fig. 6(d) we show the 30% system with a strain of 0.0015 and in Fig. 6(c) with a strain of 0.003. We note again that the overall behavior is very similar with 10%, 20%, and 30% second-phase particles, with the primary differences being the width of the transforma-
Fig. 5. System with 20% randomly placed second-phase particles (in light gray) on the microstructure used in Fig. 3. The solid lines are grain boundaries and the wide gray line is the initial crack. (a) System after a strain of 0.0015. The dark spots are transformed particles. (b) System after a strain of 0.003. (c) Stress–strain curve.

Fig. 7. System with 20% randomly placed second-phase particles (in light gray) on the microstructure used in Fig. 3. The solid lines are grain boundaries and the wide gray line is the initial crack. (a) System after a strain of 0.0015. The dark spots are transformed particles. (b) System after a strain of 0.003. (c) Stress–strain curve.

Fig. 8. System with 20% randomly placed second-phase particles (in light gray) on the microstructure used in Fig. 3. The solid lines are grain boundaries and the wide gray line is the initial crack. (a) System after a strain of 0.0015. The dark spots are transformed particles. (b) System after a strain of 0.003. (c) Stress–strain curve.
a measure of toughness, however, we see indications of a leveling off of toughness at high concentrations of transforming particles.

In the simulations just reported, we assumed a random distribution of small transforming particles, i.e. each particle was one node. An experimentally controllable parameter is, however, the size of the particles. In Fig. 9, we show results for a case where we have created larger particles by designating a node and its six hexagonally placed nearest neighbors as a transforming particle. Figure 9 corresponds to a total of 20% of all the nodes being transforming particles. We first note from the stress–strain curve that the critical stress for creation of the damage zone is 0.0019, somewhat higher than the 0.0015 needed for the case with small particles. Examination of the damage zone (Fig. 9(b)) shows that it is considerably larger than the case with the same total concentration but with smaller particles (Fig. 5). The width at a strain of 0.003 is approximately 0.45 of the cell size, considerably larger than the value (0.33) for the small particles at the same concentration. From the stress–strain curve, we find that the effective compliance is approximately 0.35, which is much larger than the value of 0.19 for the small particle case. Thus, it is clear that, by the measures used here, the material is tougher with larger particles than with smaller particles. We note that since the large particles are made up of seven nodes, the entire
Fig. 7. Stress–strain curves for the cases with 0%, 10%, 20%, 30% and 40% transforming particles.

Fig. 8. Approximate effective compliance $k_{\text{eff}}$ as defined in the text (solid line), and width of fracture zone $\Delta$, as a fraction of cell size (dashed line), as a function of the amount of second-phase particles.

Fig. 9. System with 20% randomly placed second-phase particles (in light gray) on the 100 × 100 microstructure used in Fig. 3. The particles were created as a combination of a central node and its six hexagonal nearest neighbors. The solid lines are grain boundaries and the wide gray lines are the cracks. (a) Initial conditions. (b) System after a strain of 0.0019. The dark spots are transformed particles. (c) System after a strain of 0.003. (d) Stress–strain curve.
forming particles. We are currently developing better estimates of the parameters appropriate for application to MoSi₂-based composites. Given those, more explicit predictions can be made on the optimal particle distribution.

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