FUNCTIONALLY GRADED MATERIALS: EFFECT OF ELASTIC HETEROGENEITY ON THE TOUGHNESS

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ABSTRACT

It has been demonstrated that gradients in the elastic modulus of a surface can affect the toughness of that surface [1,2]. Specifically, experimental results have correlated enhanced toughness with engineered gradients created by co-sintering a depth-dependent admixture of constituent particles with different elastic stiffnesses. While such engineered composites have average gradients that match the calculated optimal gradient, the composite microstructure will have variations in its lateral (in-surface-plane) properties and variations about the optimal gradient. The discrete nature of the particulate composites gives "stochastically graded" microstructures.

In this work, we numerically analyze the effect of stochasticity on the predicted optimal material properties and their variation. We achieve this analysis by generating a series of microstructures that have the same average surface gradient, but with variable placement of the second phase. An image-based computational tool, OOF [3] which maps material microstructures onto finite element meshes, is used to determine the local stress state. The microstructural stress is used in conjunction with a statistical representation of failure. The effect of damage accumulation on the microstructural stresses is calculated iteratively. We characterize the effect of stochastic placement of second phase particles on the toughness of these materials with a specified gradient in their surface elastic coefficients and we investigate the stability of a surface crack in such materials.

KEYWORDS

Microstructure, finite elements, functionally graded materials, Weibull statistics

INTRODUCTION

Functionally graded materials (FGM) are composites that display spatially varying properties in one thickness direction and may be characterized by spatial microstructure variations. The spatial microstructures variations are usually achieved through a non uniform distribution of the second phase and these variations can be tailored in order achieve favorable responses to prescribed thermo-mechanical loads. FGM have received recent interest due to their particular properties: functionally graded surfaces provide new microstructural designs for enhanced surface damage resistance performance in ceramic materials. In particular, Giannakopoulos et al. [1,2] demonstrated that gradients in the elastic modulus of a surface can affect the toughness of that surface. In their experimental work, enhanced toughness has been correlated with engineered gradients created by co-sintering a depth-dependent admixture of constituent particles with different elastic moduli.

In recent years, a lot of work has been carried out to study the behavior of FGM. Specifically, the finite element method has gained increasing use to determine the overall mechanical response of the materials to given solicitations. Usually FEM approaches are applied on the scale of the entire structure, the macro scale, using commercial codes such as ABAQUS (see for example [2] and [4]). On the other hand, unit cell models based on the FE analysis have been considered. However, these models cannot account for spatial variability of the constituents, due to the assumption that a structure is composed of the same microstructural representative volume element (RVE) in every part. Thus, the standard micromechanics approaches based on the concept of RVE are not suitable in the analysis of FGM, since the RVE cannot be univocally defined because of continuously changing properties through thickness. In fact, such engineered composites have average gradients that match the calculated optimal gradient on the macro scale, but the composite microstructure will have variations in its lateral properties and variations about the optimal gradient. The discrete nature of particulate composites that have been examined experimentally results in "stochastic gradients" in both microstructural directions. Neither the effect of lateral variations or perturbations about a prescribed gradient have been studied analytically.

The aim of this work is to investigate the microstructural randomness and discreteness for fixed macroscopic material gradients. Thus, a discrete computational micromechanical model is adopted. An image based finite element code, OOF, is adopted. The peculiarity of this tool is that it is able to analyze arbitrary microstructures, by mapping digitized images of microstructures and their local properties to a two-dimensional finite element mesh. In this way microstructural features can be readily modeled. To the authors' knowledge, the influence of randomness of microstructure on the macroscopic global response of FGM has been studied in literature only for the problem of thermal residual stresses [6], using a physically based micromechanics model. Here we analyze the effect of microstructural discreteness on the fracture and damage behavior of FGM, coupling OOF that calculates the local stress state with a statistical approach for brittle fracture, as described in the following section.

METHOD AND MATERIAL

As cited in the previous section, the image-based computational tool OOF is used in conjunction with a statistical representation of failure. In order to study the crack propagation, a new finite element has been implemented [7], based on a probabilistic approach for brittle fracture: the two-parameters Weibull law [8]. The microstructural mesh generation is performed using OOF and the microstructural stresses are calculated for the given loading conditions. Depending on the local probabilities of failures, this element loses stiffness as it undergoes damage and microstructural stresses are redistributed among the next elements. Thus, the effect of damage accumulation due to failure of the material can be calculated iteratively and damage can be accumulated.

The FGM considered in this study is the one experimentally characterized by Jitcharoen et al. [2]. This material is a graded alumina-glass composite whose Young modulus increases with depth beneath the surface. The thermo-mechanical properties of the constituents are summarized in Table 1.

TABLE 1

	Young modulus (GPa)	CTE (10^{-6} °C^{-1})	Poisson's ratio
Alumina	386	8.8	0.22
Glass	72	8.8	0.22

The coefficients of thermal expansion (CTE) of the two phases are approximately the same, so that thermal residual stresses do not arise upon cooling from the processing temperature.

The variation in Young's modulus of as much as 50%, introduced over a distance of 2mm, follows the law [2]

$$E(z)= E_{surface} + E_0 z^k$$

where $E_{surface}$=254GPa, E_0=85.325GPa.mm^{-k} and k=0.497, 0mm< z <2mm. The authors demonstrated that this gradient in the elastic modulus led to optimal materials properties in the contact-damage behavior.

Since we want to numerically analyze the effect of stochasticity on the predicted optimal elastic gradient, a series of "random" microstructures that have the same average surface gradient, but with variable placement of the second phase, is generated. An example is given in Figure 1 (in white alumina, in black glass).

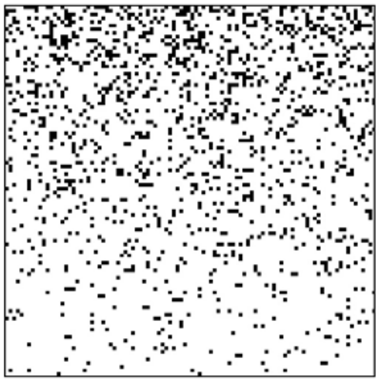

Figure 1: example of a random microstructure.

For each discrete depth z (corresponding to a layer), the Young modulus of the so represented composite can be calculated using the rule of mixtures relation

$$E_{graded}(z)= V_{glass}(z)E_{glass} + (1-V_{glass})E_{alumina}$$

where V_{glass} is the volume fraction of glass at each z. The profiles of elastic modulus were so calculated for 50 different random generated microstructures and reported in Figure 2. This picture reports the average values for each z and also average values +/- standard deviation (dashed lines). Thus a range of variability in the elastic modulus profile for real (i.e. discrete) microstructures is individuated.

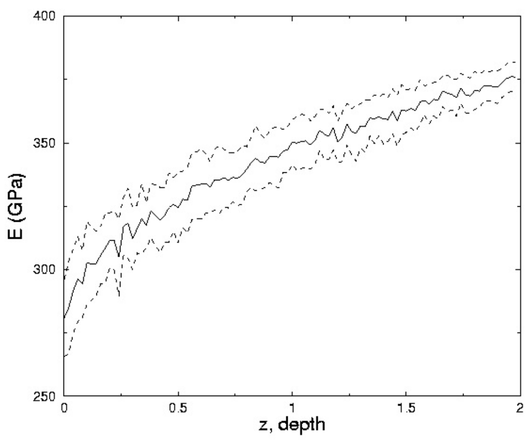

Figure 2:Young modulus vs depth z. Average values for 50 different microstructures

The average elastic modulus profile approximately coincides with that of a continuous (i.e. homogenized) material. The continuous material is achieved in this analysis generating a microstructure with several different layers, each one with a single value of elastic modulus. In the limit of an infinite number of layers, the model is continuum. An example is illustrated in Figure 3, where for clarity the number of layers has been fixed to 20.

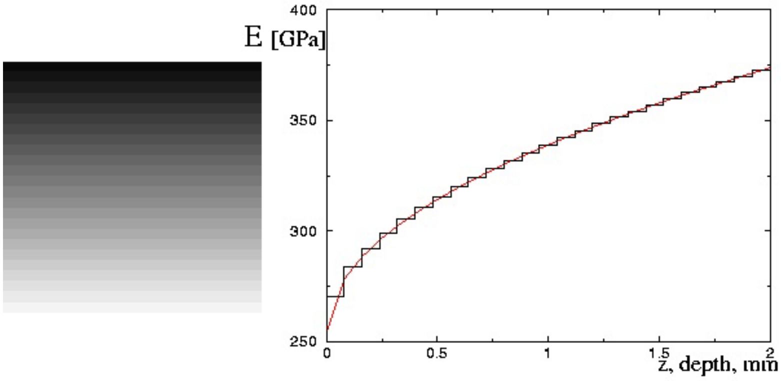

Figure 3 Continuously graded composite and corresponding Young modulus vs depth

RESULTS AND DISCUSSION

The 50 different microstructures generated as described in the previous section were meshed with OOF. Each mesh has about 20000 triangular elements. The thermo-elastic constants are known from Table 1, while the two Weibull parameters are assumed to be m=25 and σ_0=0.1GPa for both phases.
The effect of stochastic placement of the second phase on the toughness is characterized analyzing the microstructural damage evolution. We achieve this analysis placing a pre-existing surface vertical crack in each sample and incrementing the load up to the first failure. When the first element fails, local stresses are redistributed and the load can be incremented until the second failure occurs. In this manner, it is possible to track the damage evolution as the crack grows in the microstructure. Figure 4 displays the crack paths obtained for one microstructure. The elements that are damaged are colored in black.

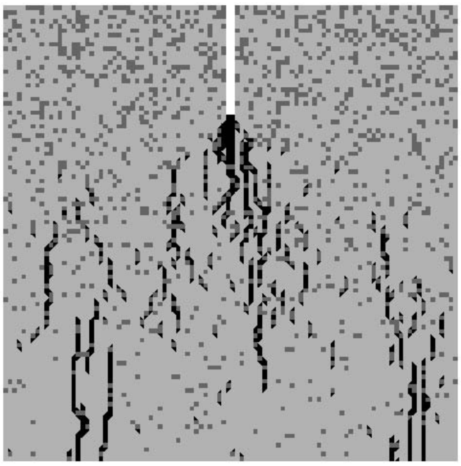

Figure 4: Damage evolution in a microstructure

In order to quantify the damage accumulation, a damage parameter has been defined as the area of the damaged elements divided by the total area. This parameter is plotted vs the strain applied in Figure 5 for one single graded microstructure and a sample of the same dimension of homogeneous material (with elastic modulus equal to the average elastic modulus through depth of the graded material). As can be noted from the picture, the sample of the graded material is less damaged, thus confirming the better performance of FGM over traditional materials.

Then, in order to quantitatively asses the effects of stochasticity of real microstructures on the fracture-damage behavior, the curves resulting from the 50 different computations have been averaged and standard deviations have been calculated. Figure 6 reports the average damage-vs-strain curve and the same curve +/- the standard deviation. The average curve (solid line) would coincide with the damage curve obtained with the continuously graded model. The two dashed curves (mean +/- standard deviation) plot how much the damage response can vary in real (and thus stochastic) microstructures. In other words, this micro-mechanic model is able to illustrate the influence of discreteness and randomness of the microstructure on the damage accumulation.

As observed also in previous studies [6], the need to consider microstructural features for modeling FGM is evident and therefore a complete micro-mechanical model should take into account the main microstructural details.

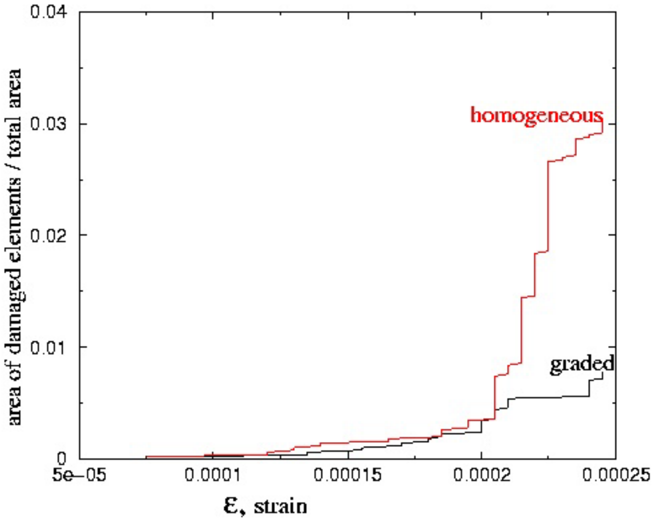

Figure 5: damage parameter for a graded microstructure and a homogeneous material

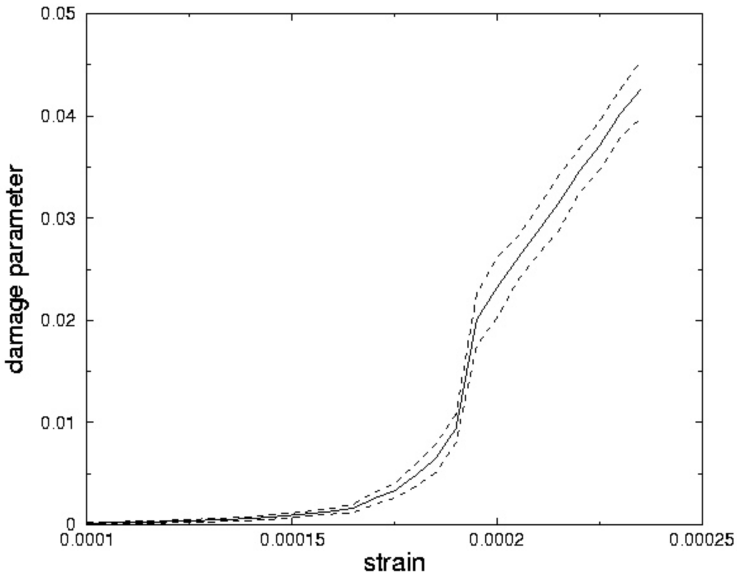

Figure 6: effects of stochasticity on the damage accumulation

Then, a new set of computations was performed on the same microstructures, but varying the Weibull moduli (m=25 for both phases, σ_0=0.34GPa and 0.06GPa for alumina and glass respectively). This choice of parameters corresponds to a realistic one for those materials, since the Weibull parameter σ_0 is a characteristic strength, related the mean fracture stress of the materials [9]. The fracture behavior in this case is different from the first set of experiments, resulting in less failures in the alumina phase where the characteristic strength is higher compared to the previous case, i.e. the damage parameter remains lower. This results underlines how the choice of the Weibull parameters, usually determined experimentally, affects the global response.

CONCLUSIONS

The focus of the paper was to analyze the effect of randomness of microstructure of FGM on the fracture-damage behavior. To this aim, a micro-mechanics model able to consider the stochasticity of placement of second phase particles is adopted: OOF, a finite element code able to operate directly on microstructural images and to create finite element meshes that take into account microstructural features, is used in conjunction with a statistical approach for brittle fracture.

The numerical analyses for the stochastically graded microstructure can be compared with those obtained for a continuous (homogeneously graded) model which does not take into account the microstructural randomness and discreteness. The results demonstrate the need to consider microstructural details for accurately modeling FGM as regards their fracture and damage accumulation behavior. In fact, the heterogeneous microstructure can affect the initiation of cracks.

This work is currently in progress. In particular, the study aims to quantitatively assess the effect of the characteristic Weibull parameter on damage accumulation. Moreover the model could be extended to account for other factors not considered in this case, such as the adhesion (strong or weak) at the interface between the two phases.

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