# A COMPUTATIONAL MODEL FOR DAMAGE EVOLUTION IN CERAMIC COATINGS: EFFECT OF RANDOM MICROSTRUCTURE

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Abstract

A novel numerical model is proposed to investigate effects of microstructure on damage and fracture evolution in ceramic coatings under mechanical loading. Random microstructures of coatings are generated by the Monte Carlo method based on the Poisson distribution of the number of microdefects and stereological size-shape distribution of voids in plasma-sprayed ceramic coatings. The initial damage distribution and corresponding effective material properties linked to the microstructures and element dimensions are determined for all elements with the use of an analytical method. Processes of failure evolution at the microscopic level are introduced into mesoscopic considerations using the framework of a continuum damage mechanics (CDM). The approach is extended to non-uniaxial stress states to describe damage evolution in the porous coatings. Initiation and growth of local microcracks linked to local failures affect damage evolution due to changes in elastic anisotropy at the level of elements and subsequent modifications of stress and strain fields. Based on the proposed algorithm, the constitutive relationship for the coatings with damage is included in the finite element code NASTRAN as an additional material subroutine. Effects of porosity, voids attributes (size, shape and numbers) of the coatings on their loading behaviours are evaluated quantitatively and qualitatively in a three point bending simulation. The results indicate that system is capable of predicting anisotropic damage growth and crack initiation in ceramic coatings.

## 1 INTRODUCTION

Ceramic coatings produced by thermal-spray deposition methods tend to have laminar microstructures including various microdefects (voids, pores and cracks). Although these defects can improve thermal-insulation properties of coatings and accommodate mismatch strains, they diminish strength of coatings and thus have a significant effect on their response to loading. Due to the complex microstructural morphology of ceramics, failure mechanisms of ceramic coatings under various loading conditions have been insufficiently understood, thus making important the extension of damage and fracture mechanics to include microstructural features of the process.

Studies of the effect of microstructure on damage evolution can be divided into three main groups: theories of effective (homogenised) media, phenomenological schemes and micro-mechanical methods. In the models of the first group, the stress-strain relationship of micro-structured damaged materials can be obtained from the analysis of corresponding undamaged materials with spatially uniform ('smeared') properties, based on the stress, strain or energy equivalence principles. In the phenomenological methods, details of the material's microstructure are indirectly described in terms of internal damage variables (of different tensorial orders), while the damage evolution is generally derived from thermodynamics. Hence, various definitions for damage and its evolution law have been proposed to describe the response of different materials to external loading [1-5]. In the micromechanical methods, the global material's response to loading and fracture evolution are studied using a direct detailed discretization of the heterogeneous microstructure for a representative volume element (RVE), assuming periodic repetition of RVEs in a macroscopic volume. In other words, the material's behaviour at the structural level is reduced to that of the RVE. Apparently, the last group of methods can more accurately describe the microstructure compared to the other two groups.

However, these assumptions are not always directly applicable to real materials of coatings. Real microstructures often demonstrate randomness in the distribution of microdefects making the periodicity assumption too restrictive. Furthermore, coatings are often directly discretized into elements in numerical simulations [6, 7], neglecting the effect of microstructure, or they are even presented as a single layer of elements with a uniform stress field [8-10], equally biaxial in the plane of the coating/substrate. In order to incorporate effective properties of brittle materials, obtained by multilevel modelling [11] or analyses at the grain level [12, 13], RVE dimensions should be much larger than a microstructural length scale. Moreover, the element size in macroscopic simulations should be at least as large as the RVE dimensions [14, 15] in order to obtain representative results. Thus, many microstructural details have to be smeared out although they could have a significant effect on damage and fracture evolution in coatings. These drawbacks are further enhanced in studies of non-uniform processes of damage and fracture in coatings under complex loading conditions as was discussed in [16] (as well as some ways to suggest more adequate models of random media).

## 2 MODEL AND RESULTS

In this paper, the effect of microstructure on local and global damage and fracture evolution in alumina coatings is examined using a finite-element description at the mesoscale. The general flow chart of the algorithm is shown in Figure 1.

In the model, random microstructures within each element of discretized plasma-sprayed ceramic coatings are accounted in terms of the Poisson distribution of the number of microdefects and their stereological size-shape distributions [17]. An example of the distribution for ceramic coatings with total porosity 5%, based on the data for the real microstructure, is given in Figure 2. Here, voids in the coating are divided into 27 discrete types, each type being characterised by a combination of a shape and size of voids. Void shapes are divided into 10 levels using a shape factor $S_{\mathrm{f}} = 1-(b/a)^2$, with its extreme values 0 and 1 corresponding to circular voids and cracks, respectively. The size $a$ (length of a major axis) of elliptical voids is divided into 8 levels starting from less than 3.3 μm up to more than 26.7 μm (*b* is a length of a minor axis). Probability $p_i$ of each type of voids in Fig.2 is determined as $p_i = r_{\mathrm{v}i}/r_{\mathrm{a}}$, where $r_{\mathrm{v}i}$ is a density of the *i*-th type of voids (defined as a number of voids in a unit area) and $r_{\mathrm{a}} = \sum_{i=1}^{27} r_{\mathrm{v}i}$ is the total void density of coating.

Then, the distribution of initial damage $D_{0\{1,2\}}$ and corresponding effective material properties (Poisson's ratio $n$ and Young's modulus $E_{0\mathrm{e}}$), linked to the microstructure and element dimensions, are determined for the material with an orthotropic distribution of elliptical voids in terms of porosity $p_{\mathrm{e}}$ and shape factors (hole density tensor **ß**) introduced in [18]:

$$E_{0\mathrm{e}\{1,2\}} = \frac{E_0}{1+p_{\mathrm{e}}+2p\{b_{11}, b_{22}\}}, \qquad (1)$$

$$D_{0\{1,2\}} = 1-\frac{E_{0\mathrm{e}\{1,2\}}}{E_0}, \qquad (2)$$

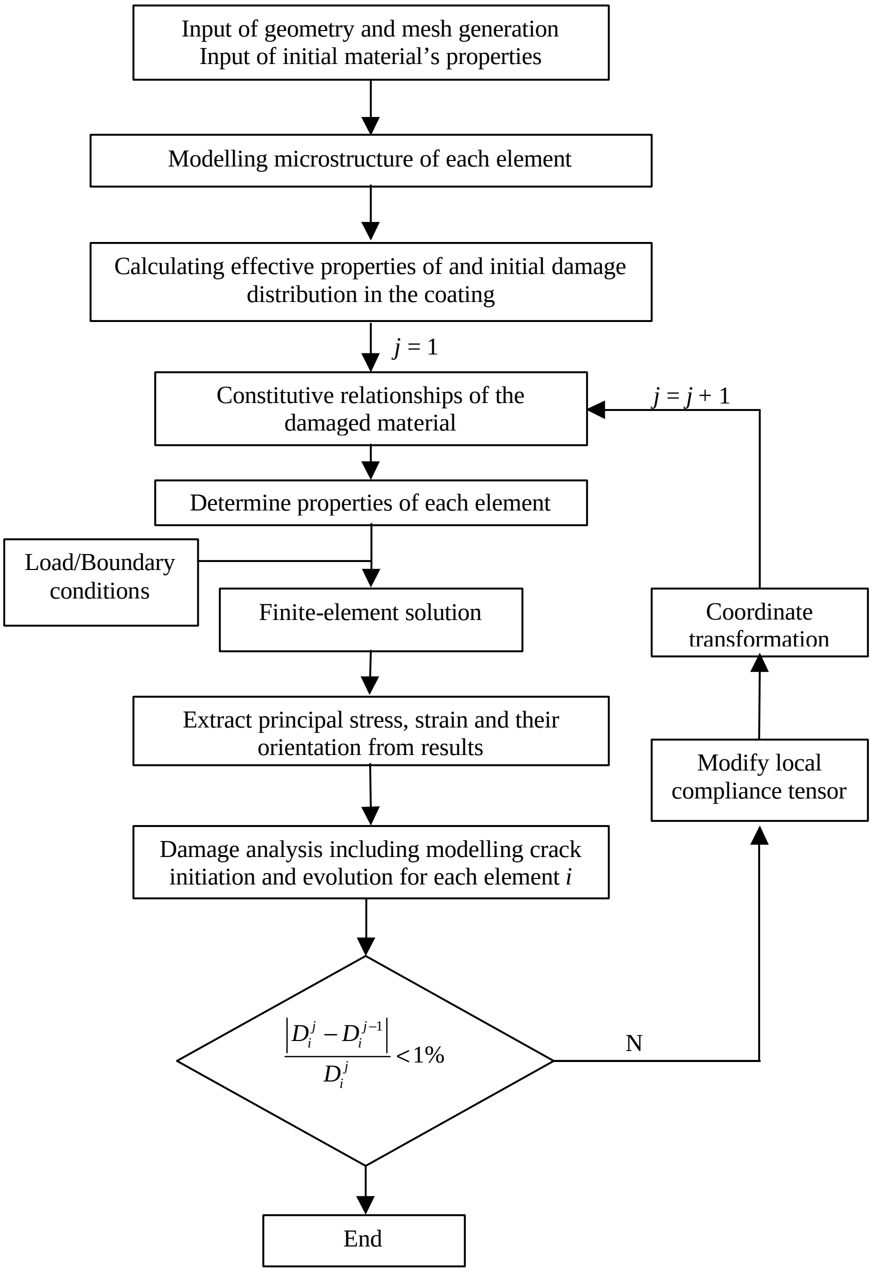


Figure 1: General flow chart of the damage and fracture analysis system

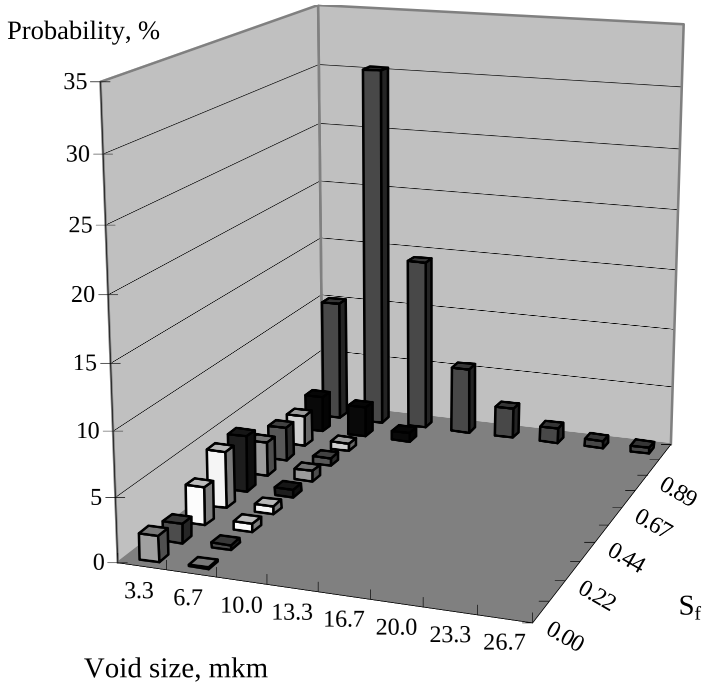


Figure 2: A shape-size-probability distribution of voids in ceramic coating

where $p_e = \frac{1}{A} p \sum_{k=1}^{n_{pi}} (a_k b_k)$ , $\mathbf{ß} = \frac{1}{A} p \sum_{k=1}^{n_{pi}} (a_k^2 \mathbf{nn} + b_k^2 \mathbf{mm})$ , $A$ is the total area, $a_k$ and $b_k$ are lengths of major and minor axes of the *k*th elliptical void, $\mathbf{n}$ and $\mathbf{m}$ are unit normals to these axes, respectively; subscript 0 refers to the undamaged material. In terms of the Poisson distribution, an exact number of the *i*-th type voids $n_{pi}$ in each element of coating with porosity *p* is determined by random sampling.

The process of failure evolution at the microscopic level is introduced into mesoscopic considerations using the framework of CDM and a damage parameter as a measure of material's deterioration. For a biaxial tensile loading state of the coating in this study, the constitutive relations for the materials with damage configuration in principal direction is expressed as:

$$s_i = \frac{E_0}{1 - n_0^2} (1 - D_i)(e_i + n_0 D_{ji} e_{ij}) = \hat{E}_0 (1 - D_i) \hat{e}_i \, , \tag{3}$$

where $s_i$ and $e_i$ ( $i, j = 1, 2;\ i \neq j$ ) are principal stresses and strains, respectively; $D_i$ is defined as damage measure induced by $s_i$ and $e_i$ in the corresponding principal direction;

$D_{ij} = \sqrt{(1-D_i)/(1-D_j)}$ accounts for the effect of damage in principal directions on the Poisson's ratio, $\hat{E}_0 = \dfrac{E_0}{1-n_0^2}$ and $\hat{e}_i = e_i + n_0 D_{ji} e_j$ represent the equivalent Young's modulus and strains, respectively. In terms of the CDM approach suggested in [5] for brittle materials with damage, $D_i$ is represented by the following relation:

$$D_i = \begin{cases} D_{0i} \exp \dfrac{\hat{E}_0 \hat{e}_i^2}{2W*} & \text{when} \quad s_i > 0 \quad \text{and} \quad \hat{e}_i > 0, \\ D_{0i} & \text{when} \quad s_i \le 0 \quad \text{or} \quad \hat{e}_i \le 0, \end{cases} \tag{4}$$

where $W^*$ is energy absorption capacity of the material [5, 19]. An element fails when the local damage attains the threshold value. In the case of such failure, it is assumed that $1 - D_1 = d_{11} << 1$. Thus, initiation and growth of local microcracks linked to local failures affect damage evolution due to changes in elastic anisotropy at the level of elements and subsequent modifications of stress and strain fields.

Based on the proposed algorithm, failure mechanisms in the alumina coating under three-point bending are investigated with the account for its microstructure. The finite-element code NASTRAN is expanded to include the constitutive relationship for a media with damage defined as a material subroutine. Effects of microstructural details of coatings including porosity, the size-shape, orientation and numbers of microdefects as well as element dimensions on the damage and fracture evolution are analysed for various cases of microstructure. One of the typical results is presented in Figure 3, which shows normalised major principal stresses, initial damage ($D_0$) and final damage ($D_1$) distribution around centre area of the coating under bending loading. The results indicate that the microstructure has a significant effect on the damage processes and failure evolution in the coating.

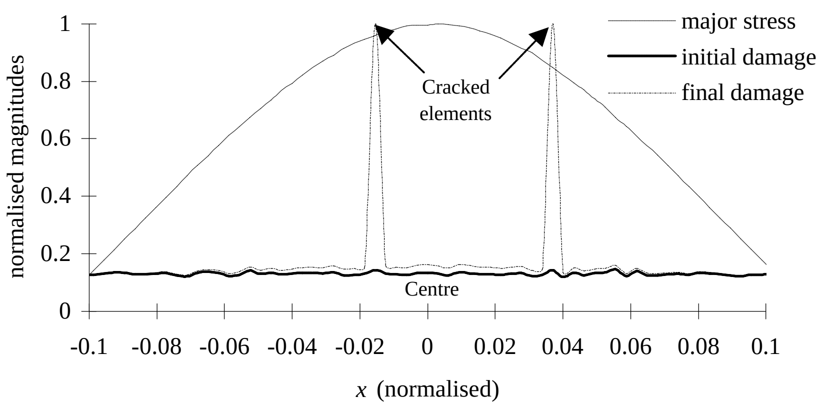


Figure 3: Effect of microstructure on damage distribution in coating's surface layer

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