Description of Brittle Behaviour of Alumina/Zirconia 2 Phase Ceramics

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Abstract. Alumina/zirconia 2 phase ceramics is innovative composite material applied for thermal barrier coatings of critical elements of jet engines. Its internal microstructure is complex as it consists of: (1) 2 phases of monolithic ceramics, (2) initial porosity and (3) other technological defects. Moreover, during loading process one can observe gradual microcracking, which is strictly connected with the loading path. The actual microstructure becomes much more complex. The crucial point in description of the behaviour of 2 phase ceramics is correlation of microcracking processes with the type of applied loading, for example: uniaxial tension, uniaxial compression or 2D and 3D states of stress. This different gradual composite degradation in tension or compression is typical for brittle materials. Here we describe both microcracking models of 2 phase ceramics associated with types of loading.

1. Introduction

Modern polycrystalline materials are created as mixture of different phases with various technological processes. Usually they have very complex internal microstructures, which include grains created from monolithic ceramic phases, system of interfaces or interphases and technological defects, e.g. [1, 2]. Examples of analytical or numerical modelling are presented in [3-14]. Modern nanoceramic composites have more complicated internal structures, e.g. [15, 16]. The similar situation is observed in case of so called functionally graded materials where the thermo-mechanical properties have continuous changes in 1 or 2 directions, e.g. [17-28]. Typically, ceramic matrix composite (CMC) consists of elastic phases. However, in case of advanced ceramic materials like cerments, interphases or interfaces between elastic grains are plastic e.g. [29-40].

Estimation of the overall properties of heterogeneous materials were described in [41-47]. Postulation existence of the Representative Volume Element (RVE) in microscale and assumption of statistical homogeneity of the CMC allows for formulation of general results relating to bounds of micropotentials and strain as well as complementary energies functionals. Assessment of the complex composites response containing: (1) different phases, (2) impurities and (3) different kinds of structural defects (dislocations, pores, cracks etc.) inside the material is possible by application of averaging procedure over the RVE.

The analysed alumina/zirconia ceramics can have different volume contents of both phases. However, the experimental investigations were done for small amount of zirconia up to 20%. To describe brittleness of the ceramic composite we considered different states of loading and cracks.
propagation processes under pure tensile or compression. The matrix material is Al₂O₃ (phase I), whereas the phase II, i.e. ZrO₂ has different thermal expansion coefficient what causes initiation of small amount of microcracks and micropores during technological cooling. These initial microdefects cause stress concentrations, when material is subjected to loading. Microdefects can develop to longer mesocracks and finally can create dominant macrocracks leading to polycrystalline ceramics failure. We applied mesoscale model, using averaging procedure over the Representative Surface Element (RSE), for description of different cracking phenomena at micro- and meso- scales, which developed during different deformation stages.

2. Micromechanical model for 2 phase ceramic polycrystalline composites

Figure 1 presents advanced stages of deformations of the Al₂O₃/ZrO₂ polycrystalline ceramics with system of initial defects (e.g. pores, microcracks etc.) and developed complex state of different types of cracks. The whole deformation processes in analysed ceramics associated with nucleation and growth of different defects can be described as sequences of the following stages:

- creation of initial defects during technological cooling – micropores and microcracks are distributed inside grains or grain boundaries due to mismatch of the thermal expansion coefficient of 2 phases creating the composite polycrystal,
- development of initiated microcracks by their growth along the nearest grain boundaries due to the fact, that grain boundaries have lower value of fracture resistance in comparison to grains. This process ends in creation of mesocracks, which occupy the whole straight segment of grain boundaries,
- creation of the wing cracks when mesocracks start to kink and spread along the sequent segment of the polycrystalline grain boundaries system. In advanced stages of pure tensile or compressive deformations the polycrystalline material has complex internal structure, figure 1a and 1b.

![Figure 1. Advanced stage of deformation of the Al₂O₃/ZrO₂ polycrystalline ceramics - cracked microstructure due to a) compression, b) tension](image)

All the above described stages of deformation can be expressed by the following constitutive equations using Voigt notation:

\[
\{\varepsilon_i\} = \{\bar{S}_{ik}^{\text{CMC}}(\sigma_{ik}, p_{ZrO_2}, p_o, N^{(6)})\} \{\sigma_k\}
\]

for \(i,k = 1,...,6\). In (1) \(\{\varepsilon_i\}\) denotes the strain vector, \(\{\bar{S}_{ik}^{\text{CMC}}\}\) is the averaged elastic compliance matrix, \(\{\sigma_k\}\) is the stress vector. Moreover, \(p_{ZrO_2}\) is the volume content of the second phase (ZrO₂), \(p_o\) is the
initial porosity parameter and \( N^{(i)} \) are sets of numbers defining different kinds of discontinuities “s” developing inside the material, figure 1a and 1b.

In the advanced state of deformation the averaged elastic compliance tensor \( \{ \overline{S}_{ik}^{\text{CMC}} \} \) can be decomposed to:

\[
\{ \overline{S}_{ik}^{\text{CMC}} (\sigma_r, p_{ZrO_2}, p_o, N^{(s)}) \} = \left\{ \begin{array}{l}
(1 - p_{ZrO_2} - p_o) \{ S_{ik}^{\text{Al}_2\text{O}_3} \} + \\
+ p_{ZrO_2} \{ S_{ik}^{ZrO_2} \} + \\
+ \{ S_{ik}^o (p_o) \} + \\
+ \sum_{(s)} \{ S_{ik}^{(s)} (\sigma_r, p_{ZrO_2}, p_o, N^{(s)}) \}
\end{array} \right. .
\]

\( \{ S_{ik}^{\text{Al}_2\text{O}_3} \} \) is the compliance elastic matrix of the matrix material \( \text{Al}_2\text{O}_3 \), \( \{ S_{ik}^{ZrO_2} \} \) describes the elastic properties of the \( \text{ZrO}_2 \). \( \{ S_{ik}^o (p_o) \} \) is the part of the compliance elastic matrix related to the existence of the initial porosity. The last part of (2) includes all different types of defects (micro-, meso- and macrocracks) inside the RSE.

The third part of the averaged elastic compliance tensor (2) \( \{ S_{ik}^{(s)} (p_o) \} \) describes initial porosity of the ceramic matrix composite. This part was estimates in [47] as:

\[
\{ S_{ik}^{(s)} \} = \left[ \begin{array}{cccc}
3/4 & -1/4 & -1/4 & 0 & 0 & 0 \\
-1/4 & 3/4 & -1/4 & 0 & 0 & 0 \\
-1/4 & -1/4 & 3/4 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{array} \right] \frac{4[1 - (v_o^{\text{CMC}})^2]}{E_o^{\text{CMC}}} \left[ \begin{array}{c}
p_o \\
1 - p_o
\end{array} \right] .
\]

Here \( E_o^{\text{CMC}} \) and \( v_o^{\text{CMC}} \) are the Young’s modulus and the Poisson’s ratio of the initial polycrystalline ceramics without porosity.

As it is seen in figure 1, in the advanced stages of deformation one can distinguish the following types of defects, which appear inside the material: (1) opened mesocracks, (2) closed mesocracks, (3) wing cracks with opened central part, (4) wing cracks with closed central part.

Following [48-50] we can formulate constitutive equations for calculation of the averaged strain vector \( \{ \overline{\varepsilon}_{ik}^{\text{me}} \} \) and the compliance matrix \( \{ \overline{S}_{ik}^{\text{me}} \} \) for single active opened mesocracks “s” developed inside the RSE:

\[
\{ \overline{\varepsilon}_{ik}^{\text{me}} \} = \sum_{(s)} \{ \overline{S}_{ik}^{\text{me}(s)} \} \{ \sigma_{ik} \} = \int_{D_m} \int_{\phi^{(s)}} M_{\nu}^{\text{mc}} (\phi^{(s)}) \sigma_j (\phi^{(s)}) p_1^{\text{mc}} (\phi^{(s)}) \left[ \begin{array}{cccc}
D & 1/4 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array} \right] \frac{2\pi}{A E_o^{\text{CMC}}} N^{\text{me}}_o .
\]

where \( N^{\text{me}}_o \) is a number of active mesocracks in the RSE of the area \( A \). \( D \in (D_m, D_M) \) and is the size of the grains inside the RSE. \( D_m \) and \( D_M \) are maximum and minimum value of grains diameters in the RSE. \( M_{\nu}^{\text{mc}} (\phi^{(s)}) \) is the matrix describing functions of inclination \( \phi^{(s)} \) of the mesocracks “s” in relation to horizontal axis, figure 2. \( p_1^{\text{mc}} (\phi^{(s)}) \) is the distribution function of the mesocracks inclination angle \( \phi^{(s)} \). \( p_2^{\text{mc}} (D) \) denotes the distribution function of grains length.

In case of closed mesocracks it is necessary to include friction coefficient \( \mu \) along the cracks length, i.e. function \( M_{\nu}^{\text{mc}}(\phi^{(s)}, \mu) \) depends on 2 variables, e.g. [48-50].
The wing cracks are presented in figure 2. They consist of 1 central mesocrack and 2 wings. For example, the mechanical response of mesocracks creating wings and additional strains due to wings opening for the tension (figure 2b) can be expressed by:

\[
\{ \varepsilon^{\infty} \} = \left[ \frac{\partial_{ij} \phi^{(s)} \sigma_{ij}(\phi^{(s)}) p_{ij}^{(s)}(\phi^{(s)})}{\sigma_{ij}^{(s)}} \left( \frac{D}{4} \right)^{2} p^{(s)}(D) \, d\phi^{(s)} \, dD \right] \frac{2\pi}{AE_{mc} N_{j}^{mc}} \cdot (5)
\]

Here, \( \{ \varepsilon^{\infty} \} \) is the averaged strain vector, \( N_{j}^{mc} \) denotes a number of the wing cracks inside the RSE. \( M_{ij}^{mc}(\phi^{(s)}) \) is the matrix describing mesocracks which are able to create 2 wings at their tips, \( M_{ij}^{mc}(\phi^{(s)}, \theta^{(s)}) \) - the matrix of spatial placement of the wing “s”. \( \phi_{1}^{mc} \leq \phi^{(s)} \leq \phi_{2}^{mc} \) is the fan of all mesocracks creating wings, \( p_{ij}^{mc}(\phi^{(s)}) \) - is the distribution function of the active mesocracks creating wings. \( D/2 = 2c^{(s)} \) is the length of the straight grain boundary segment. \( p^{(s)}(D) \) is the distribution function of \( D \). \( T^{(s)} = t^{(s)} / c^{(s)} \) - is the nondimensional wing length, \( \bar{l}^{(s)} \leq T^{(s)} \leq \bar{L}^{(s)} \) - is the fan of the wings lengths inside the RSE. \( \theta_{1}^{mc} + \theta_{2}^{mc} \leq \theta^{(s)} + \theta^{(s)} \leq \theta_{2}^{mc} + \theta_{2}^{mc} \) is the fan of inclination angles of the wings. \( p_{ls}(\bar{l}^{(s)}) \) and \( p_{ls}(\theta^{(s)} + \theta^{(s)}) \) are the distribution functions of the wings lengths and the inclination angles.
For the wing crack models with closed mesocrack (figure 2a) it is necessary to include friction coefficient $\mu$ and the functions: $M_{cm}(\phi^{(0)})$ and $M_{c}(\phi^{(0)}, \theta^{(0)})$ should be replaced by $M_{cm}(\phi^{(0)}, \mu)$ and $M_{c}(\phi^{(0)}, \theta^{(0)}, \mu)$, respectively.

In order to describe the set of cracks development inside the RSE we used the strain energy release rate criterion. For one closed mesocrack or the wing crack we have:

$$ G^{(i)} = \begin{cases} G^{cm}(\sigma_c, c^{(0)}, \phi^{(0)}) \\ G^{c}(\sigma_c, c^{(0)}, \phi^{(0)}, \mu) \\ G^{cm}(\sigma_c, c^{(0)}, \phi^{(0)}, \theta^{(0)}) \\ G^{c}(\sigma_c, c^{(0)}, \phi^{(0)}, \theta^{(0)}, \mu) \end{cases} = \frac{1}{K_{\phi}^{CMC}} \left( K_I^2 + K_H^2 \right) \geq 2J_{\phi}^{CMC}, \quad (7) $$

where, $G^{cm}(\sigma_c, c^{(0)}, \phi^{(0)}, \mu)$ and $G^{c}(\sigma_c, c^{(0)}, \phi^{(0)}, \theta^{(0)}, \mu)$ are the strain energy release rate function for the mesocrack “s” or the wing crack. $\gamma_{\phi}^{CMC}$ is the surface energy between grain boundaries of the polycrystalline composite. In case of the opened mesocracks or the wing crack we have functions $G^{cm}$ with $\mu = 0$. The analysis of crack kinking to the nearest grain boundary was presented for example in [51-62], but with application of numerical models. $K_I$ and $K_H$ in (7) are stress intensity factors in tips of propagating cracks. They can be expressed for the single crack as:

$$ K_I = \begin{cases} -D \left[ \sin \phi^{(0)} \left( \cos \phi^{(0)} - \left( \frac{\mu = 0}{\mu \sin \phi^{(0)}} \right) \sin \theta^{(0)} \right) \left[ \pi \left( l^{(0)} + l' \right) \right] ^{(l/2)} \right] + \\ + \left( \pi l^{(0)} \right)^{(l/2)} \frac{1}{2} \left[ 1 - \cos 2(\theta^{(0)} + \phi^{(0)}) \right] \right] \right] \sigma_1, \quad (8) $$

$$ K_H = \begin{cases} D \left[ \sin \phi^{(0)} \left( \cos \phi^{(0)} - \left( \frac{\mu = 0}{\mu \sin \phi^{(0)}} \right) \cos \theta^{(0)} \right) \left[ \pi \left( l^{(0)} + l' \right) \right] ^{(l/2)} \right] + \\ + \left( \pi l^{(0)} \right)^{(l/2)} \frac{1}{2} \sin 2(\theta^{(0)} + \phi^{(0)}) \right] \right] \sigma_1. \quad (9) $$

In case of the opened mesocracks or wing cracks with opened central part $\mu = 0$. Moreover, $l^{(0)} + l'$ is so called equivalent length of wings, e.g. [41, 63].

3. **Numerical results**

To illustrate level of brittleness of the considered ceramic composite $\text{Al}_2\text{O}_3/\text{ZrO}_2$ we discussed tension and compression deformation processes. Both composite components: $\text{Al}_2\text{O}_3$ and $\text{ZrO}_2$ are characterized by the following initial properties:

- $\text{Al}_2\text{O}_3$ – the Young’s modulus $E_0 = 400$ GPa and the Poisson’s ratio $\nu_0 = 0.22$ and the fracture toughness $K_c = 4.5$ MPam$^{1/2}$,
- $\text{ZrO}_2$ - the Young’s modulus $E_0 = 200$ GPa and the Poisson’s ratio $\nu_0 = 0.25$ and the fracture toughness $K_c = 10$ MPam$^{1/2}$.

The mean diameter of the CMC structure was $10^{-5}$ m, whereas $D_m = 8 \cdot 10^{-6}$ m and $D_M = 12 \cdot 10^{-6}$ m.

Figure 3 presents deformation processes under compression and tension for composite including 10% and 20% ZrO2. Characteristic points corresponding to the mesocracks and the wing cracks are specified. Application of the second phase (ZrO$_2$)leads to decrease of the load capacity of the Al$_2$O$_3$, however, increases its deformability and the fracture toughness. The compressive strength is approximately 10
times higher in comparison to tension. Additionally, a comparison with performed experiment confirms applicability of the model to modelling of the 2-phase CMCs. The experiments were done with sample of diameter 6 mm and height 20 mm with testing machine MTS 250 kN.

![Graph](image)

**Figure 3.** Deformation processes of the ceramic composite for: a) compression and b) tension

4. **Final remarks**

Performed numerical analysis and experimental tests with Al$_2$O$_3$/ZrO$_2$ ceramic composite lead to the following conclusions:

- The brittle behaviour of the composite is strong.
- Level of the volume contents of: (1) ZrO$_2$ and (2) porosity strongly influence the material behaviour under mechanical loading.
- Microcracks develop under mixed mode of fracture along straight segment of grain boundaries to form mesocracks,
- Further growth of the mesocracks is by intergranular kinking to form the wing cracks.
- The dominant wing cracks can develop by intergranular or transgranular manner leading to the composite failure.

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