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INFLUENCE OF PHASE TRANSFORMATION ON SUBCRITICAL CRACK GROWTH IN NUMERICAL MODELLING OF A CERAMIC COMPOSITE

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ABSTRACT

The aim of the work is to establish the method of numerical simulation of stress induced transformation of ZrO_2 from the tetragonal to monoclinic phase which takes place at the crack tip in two-phase Al_2O_3– ZrO_2 ceramic composite. It is the base for the future crack growth numerical simulations in composite with the use of FEM models with the real grain size distribution and shape. The preliminary analysis allows us to estimate influence of phase transformation of the composite on the cracking resistance.

KEYWORDS

Al_2O_3, ceramic composite, ZrO_2 phase, phase transformation, crack propagation, FEM (Final Elements Method)

INTRODUCTION

Due to their properties, such as high chemical corrosion resistance, high temperature resistance, relatively low density and high hardness as well as shear strength, ceramic materials make a very interesting material for design engineers. They are not widely implemented only because of their brittleness and low cracking resistance. Therefore, many laboratories all over the world have been carrying out intensive research to fully explain the nature of crack formation in ceramic materials. However, this phenomenon still remains far from being explained even in case of single phase Al_2O_3 ceramic material which probably is the most widely tested one.

The issue which attracts researchers' attention is the increase in the material cracking resistance as a function of the crack growth length (R-curve or T-curve). This was observed in case of Al_2O_3 ceramics, Al_2O_3 ceramics with SiC whiskers, corundum ceramics with ZrO_2, stabilized zirconium ceramics, and silicon nitride ceramic materials.

Two theories are used to describe the problem. The first is the theory of bridges created behind the tip of the surface crack. This theory is especially helpful for the description of crack resistance feature of a material which does not undergo stress induced phase transformation. The material which can be best analysed in this way is, for example, pure corundum ceramics.

Another theory used in the analysis of materials containing phases which undergo transformation on the phenomenon of the formation of phase transformation zone surrounding. It is induced by local stress areas developing in front of the crack tip during the crack growth. The direction of tensile stresses is perpendicular to the direction of crack propagation and compressive stresses appear in the direction which is parallel to the crack.

The zirconium dioxide placed in the aluminum oxide matrix with high Young module is compressed in the areas which are distant from the head of the crack. The field of tensile stresses which develops ahead of the developing crack induces the tetragonal zirconium phase and allows for its change into the monoclinic phase with different shape and larger volume. As the result the crack tip stresses are reduced and the cracking resistance increases. This leads to the formation of transformed phase layer along the crack surface.

It is commonly assumed that the thickness of the transformation layer is constant. The thickness is determined by the matrix cracking resistance and the stresses enabling the process of transformation regardless of the tetragonal phase grain size. It is possible that the thickness of the transformation layer depends on the tetragonal phase grain size. There exists a correlation between the growth in the transformation layer and the cracking resistance increase.

The assumption concerning the stress decrease in the area of the crack tip as a result of the process of phase transformation has been used by Evans [1, 2] who has suggested an expression defining the relation between the cracking increase, transformation layer thickness and the crack growth in the transformation zone:

$$\Delta K_I = \frac{Ee^T V_f \sqrt{w}}{1-\nu} \kappa(\Delta a / w, \nu) \tag{1}$$

where

E is the Young module of the matrix containing zircon dioxide,

e^T is the transformation strain,

V_f is the volume of the transformed grains,

ν is Poisson's ratio,

κ is the function the value of which increases with the crack growth, describing the material cracking resistance.

Both the „zone" and the „bridge" theory, lead to the conclusion that the stress intensity coefficient K_{Itip} in the crack tip can be written as follows:

$$K_{Itip} = K_{Ia} - K_{Is} \tag{2}$$

where K_{Ia} is the stress intensity coefficient used, K_{Is} is the „shielding" stress intensity coefficient which grows in relation to the crack length until its maximum value $K_{IS_{max}}$ is reached.

The speed of the crack growth is usually described by the following dependence:

$$V = da / dt = A(K_{Itip})^n \tag{3}$$

where A and n are subcritical cracks growth parameters. Because K_{Ia} (where Y is constant depending on the geometry of the analysed system with a fault, σ_a is the stress applied) it may turn out that in some range of values (for $\sigma_a < \sigma_c$, where σ_c is the strength of the material) the increase of the K_{Is} value in the a function will exceed K_{Ia}. This will lead to the retardation of the crack propagation. There is then a possibility of minimizing the phenomenon of subcritical cracks growth which are responsible for the unexpected damage of the ceramic construction elements. If some parameters of the microstructure are known, i.e. the grain size, mechanical properties determined by the Young's module E, the Poisson's ratio ν, resistance σ_c, cracking resistance K_{Ic} , corresponding to the length of the „natural" flaw, it is possible to calculate numerically the run of the R or T curve. This in turn, allows for defining the range of the flaw sizes if $\sigma_a < \sigma_c$ for which the growth of subcritical cracks is reduced to minimum.

The work on the creation of numerical models, calculation methods, results analysis and evaluation can be basically applied into two areas: the area of ceramic materials without the phases undergoing transformation and the area of materials containing the phase which undergoes transformation. The main stages of the experimental and numerical research within these areas are similar.

On the basis of numerical simulation both the R and T curves as well as the dependence of subcritical cracks growth speed rate V on the stress intensity coefficient can be determined for both types of ceramics. The lifetime, that is the time of use of a given construction element made of the above mentioned type of ceramics including a fault causing stress concentration (such as a crack, cut, Vicker's impression) can also be determined.

PHASE TRANSFORMATION SIMULATION TEST

In earlier works authors established methods for residual stress state numerical assessment and for bridging effect simulations with finite elements method (FEM) [9,10,11,12]. The residual stress state was investigated for the pure Al_2O_3 ceramics as well as for Al_2O_3–ZrO_2 composites with the use of 3D models. For composite containing 20% of ZrO_2 there were obtained values of average residual stresses of ~+700 MPa and ~–250 MPa respectively for ZrO_2 and Al_2O_3 phases (for temperature decrease ΔT = -1150º) which are comparable with example references [7, 8].
The application of numerical modelling results in the creation of the models describing the effect of the phase transformation at the tip of the growing crack.

For the need of phase transformation simulation method establishing 2D models of microscopic volume of two phase polycrystalline material (e. g. composite on base of Al_2O_3 and ZrO_2) were created and tested. The models containing octagon and square grains allow for making simulations for different volume fractions of Al_2O_3 and ZrO_2. As an example the mesh for the model of the material containing 20% of ZrO_2 (simulated by square grains) is presented in Figure 1. Such a mesh containing ideal grains which are uniform for each phase may be treated as "geometrically averaged" (in the sense of size, shape and topology). It is useful for making global observations, which are not affected by a number of factors that take effect in the real material (e. g. distribution of size and shape of grains). This coarse mesh is destined for tests which may answer the question: whether the FEM modeling is able to simulate phase transformation or not.

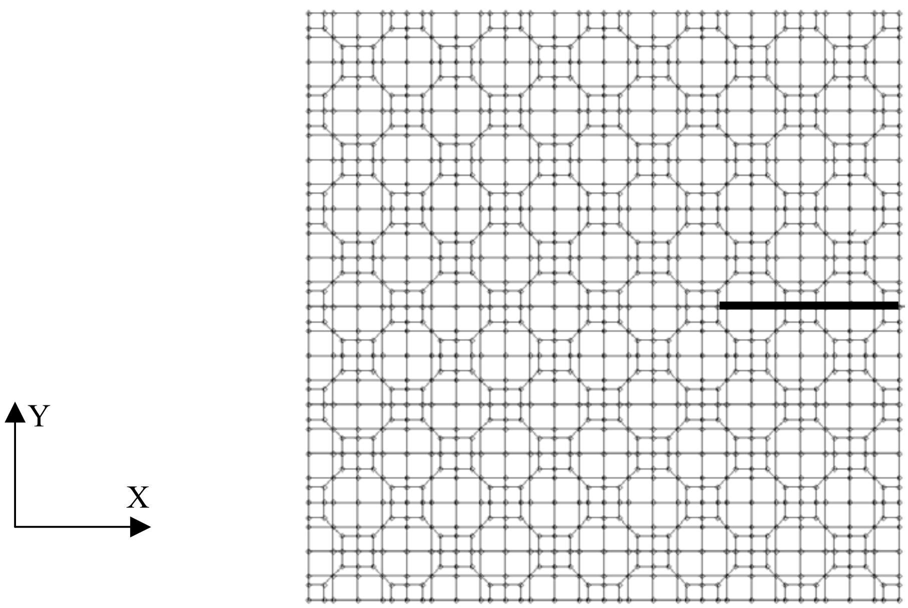

Figure 1: The mesh of the 2D model of two phase polycrystalline material taken for testing calculations. The area fraction of squares is 20%. The bold line shows the crack simulation.

The properties of the phases taken into numerical tests were found mainly in references [13,14]. They are collated in the Table 1. It was assumed that the temperature decrease was $\Delta T = -1500°$. The model is also loaded by displacements of the model boundaries, complying with thermal contraction of surrounding volume of material which in macro scale behaves like isotropic, totally homogeneous one, characterized by thermal expansion coefficient $\alpha_{iso\text{-}MACRO} = 9.3$ placed in Table 2. Values in Table 2 are the weighted sum of appropriate values from Table 1 with respect to volume fractions of Al_2O_3 and ZrO_2.

TABLE 1

MATERIAL PROPERTIES FOR PURE CERAMICS

	Al_2O_3	ZrO_2
E [GPa]	400	200
ν	0.23	0.32
$\alpha_a = \alpha_m$ $[K^{-1}]$	8.6 e^{-6}	9.2 e^{-6}
α_c $[K^{-1}]$	9.5 e^{-6}	10.75 e^{-6}
α_{izo} $[K^{-1}]$	8.9 e^{-6}	10.9 e^{-6}
$\Delta\alpha_{\alpha c\text{-}\alpha a}$ $[K^{-1}]$	0.9 e^{-6}	1.55e^{-6}

TABLE 2

MATERIAL PROPERTIES FOR THE AL_2O_3 + 20% ZRO_2 COMPOSITE - EQUIVALENT FOR MACRO LEVEL

Material	E_{MACRO} [GPa]	ν_{MACRO}	$\alpha_{iso\text{-}MACRO}$ $[K^{-1}]$
Al_2O_3 + 20% ZrO_2	360	0.25	9.3e^{-6}

In preliminary tests thermal orthotropy of materials is not considered yet. It means that the model grains of Al_2O_3 and ZrO_2 have appropriate isotropic properties ($\alpha_{iso\text{-}MICRO}$) shown in Table 1. This is because the residual stress effect caused by random orientations of material axes in neighboring grains would make it difficult to detect (in the model) the phase transformation phenomenon itself. Random orientation of orthotropy axes in particular model grains - with appropriate orthotropic thermal expansion coefficients - will be then allowed in succeeding simulations.

In preliminary tests an external uniaxial tensile load in the direction perpendicular to the plane of the crack was introduced too. It induces stress σ_y (in the global coordinate frame) on the level of 160 MPa. Such a load causes initial opening of the modeled crack tip.

To recapitulate – the complete set of loads contains: temperature decrease ΔT, displacements of the model borders simulating contraction of the macroscopic environment and the external uniaxial tensile load initializing the crack tip opening.

Figure 2 shows σ_y stress state at the crack tip in the model while the load consists of external uniaxial tension, temperature decrease $\Delta T = -1500$ and the contraction of the macroscopic environment. The crack tip is still open (the scale for displacements: 30:1 – large enough to observe crack tip opening). The stress concentration in the grain of ZrO_2 placed at the crack tip reaches maximum value $\sigma_y \approx +865$ MPa.

Figure 3 shows σ_y stress state at the crack tip in the model while the load consists of uniaxial tension, temperature decrease $\Delta T = -1500$ and the contraction of the macroscopic environment. The phase transformation is simulated in all the grains in the model by the thermal coefficient correction from 10.9e-6 to 10.8e-6 K^{-1}. The crack tip is constrained to be closed. The grain of ZrO_2 placed at the crack tip is then under tensile stress, the maximum value of their concentration decreased to the value $\sigma_y \approx +806$ MPa (the stress relaxation effect induced by phase transformation simulation is visible).

Different shapes and ranges of phase transformation zones were tested to investigate sensitivity of the FEM model: from the case of the zone containing only one monoclinic ZrO_2 grain at the crack tip to the case in which all the grains in the model were transformed. Increasing the dimensions of phase transforming zone in the model produces more and more visible effect of crack tip closing and stress concentrations decrease in transformed grains. The FEM model behaves properly in the qualitative sense.

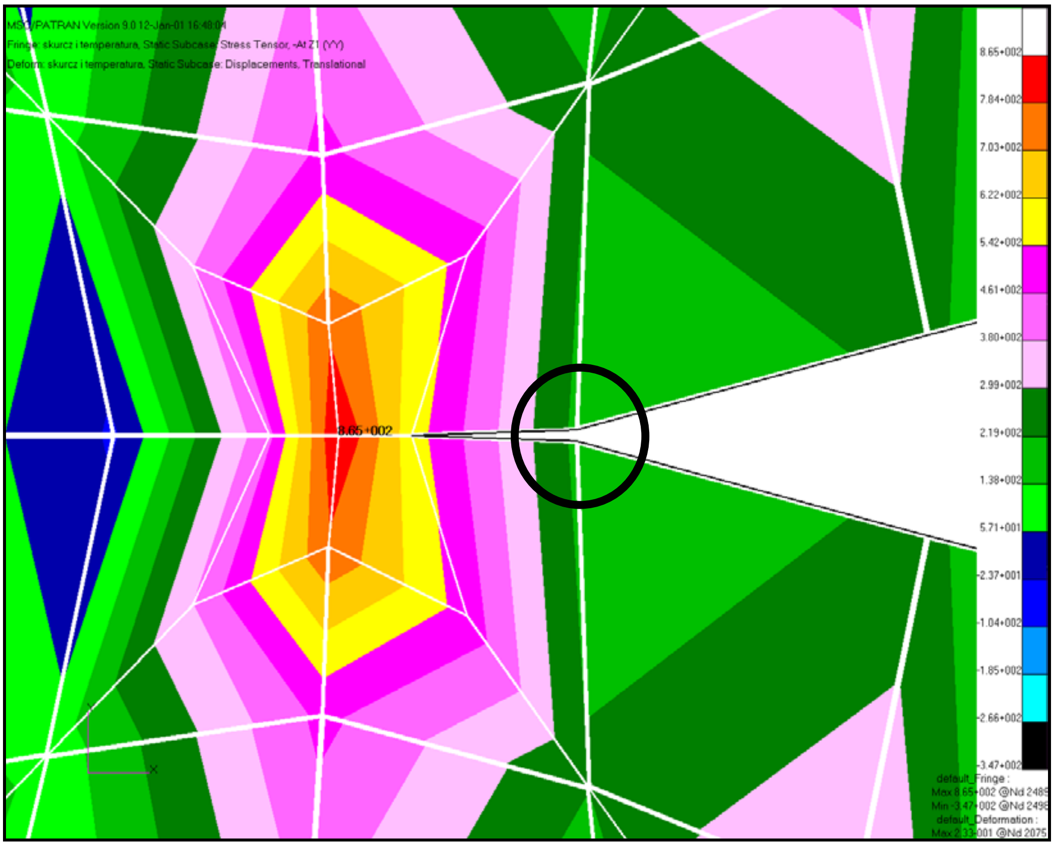

Figure 2: σ_y stresses at the crack tip while the load consists of external uniaxial tension, temperature decrease $\Delta T = -1500$ and the contraction of the macroscopic environment. The crack tip is still opened due to the external uniaxial load (the scale for displacements: 30:1).

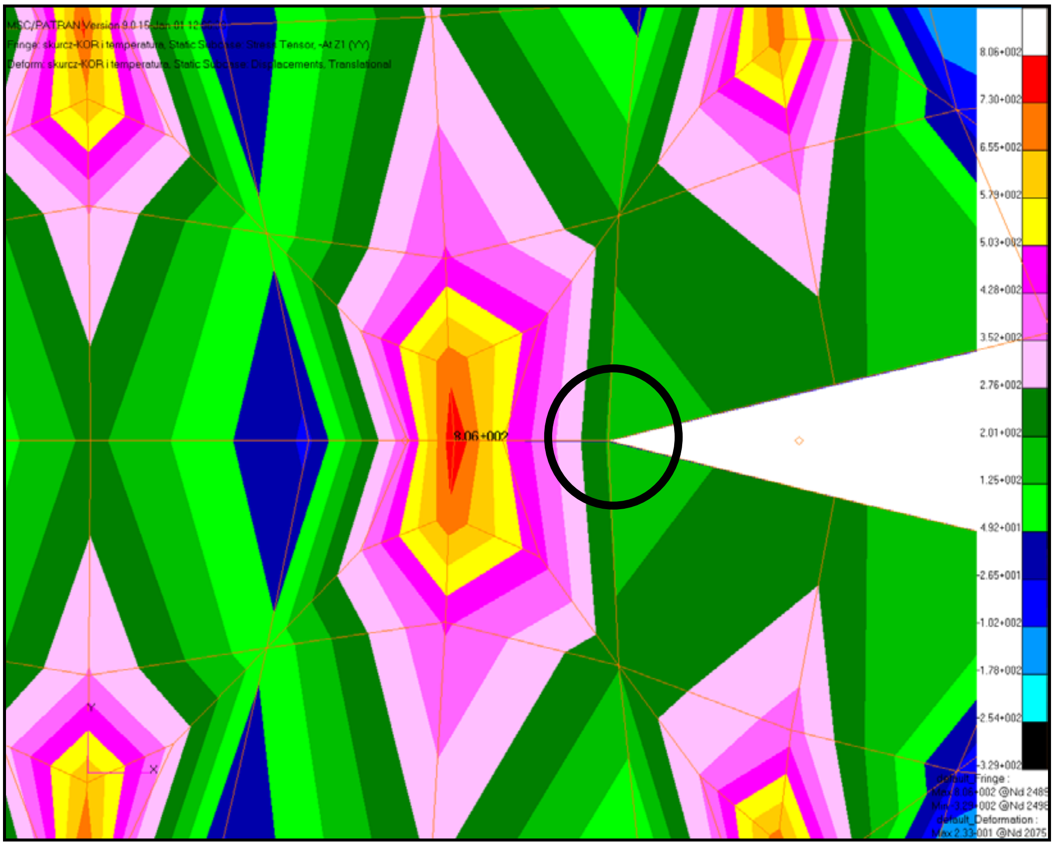

Figure 3: σ_y stresses at the crack tip while the load is the same like in the previous case but the phase transformation is simulated in all the grains in the model. The crack tip is constrained to be closed (the scale for displacements: 30:1).

CONCLUSIONS

The values of stresses obtained for 2D FEM models are comparable with those obtained with the use of 3D ones which were applied earlier for residual stresses assessment [9,10,11,12] and with references [7,8]. Preliminary tests show that FEM modelling of phase transformation phenomenon in $ZrO_2 + Al_2O_3$ ceramic composite is possible. It may be achieved by thermal expansion coefficient correction, equivalent to difference in specific volumes of tetragonal and monoclinic phases of ZrO_2. The tests presented in the paper may be now completed by consideration of random orientations of thermal orthotropy axes in neighboring grains. Presented work is the base for numerical investigations with the use of FEM models with finer meshing, complying with the experimental microscopic observations.

The novelty of this kind research is reflected by the fact that our methods of the numerical simulation will assist the experimental research, speed up the research process and will aid the design of ceramic construction elements while taking into consideration real loads. The results obtained can also reflect the grain size of the ceramic microstructure, the influence of the two types of phenomena on the crack propagation which occur in the crack zone in two kinds of the ceramic material, namely the „bridge" phenomenon (in the pure corundum ceramics) and the phase transformation (in the zircon dioxide ceramics).

The methods which have been worked out and experimentally verified allow for the crack resistance analysis of the real construction elements made of brittle kinds of ceramics used in real conditions and loads (e.g. heat load). The authors of the method believe it will find a wider application in assessing cracking resistance of various kinds of polycrystalline brittle materials with „bridge" or phase transformation effects.

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