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RESIDUAL STRESS CONCENTRATIONS ASSESSMENT IN CERAMICS USING FEM

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ABSTRACT
The paper discusses the determination of residual stress state in a cooled down orthotropic alumina ceramics with the use of FEM (finite elements method) numerical modelling. The discrete model takes into consideration the ceramics consisting of two dominating grain size fractions. The current model allows changing the proportion between grain sizes in the fractions. The results of computations are presented as distributions of the residual stress components. The stress concentration areas are responsible for cracks origination and path determination of their subcritical growth. The average value of the stress component σ_c is identified as the peak position of the proper distribution and it is quantity characteristic for a given ceramics. The presented model may be used for investigation of ceramics and ceramic composites as well.

KEYWORDS
Orthotropic microstructures, alumina ceramics, numerical modelling

INTRODUCTION

In cooling down polycrystalline alumina from sintering to room temperature the random variation in crystallographic orientation of orthotropy from one grain to another induces a very complex state of constraint. This leads to appearing and remaining of the complex three-dimensional residual stress state in the ceramic material at the room temperature. Stress concentration areas have fundamental significance for strength property, especially for the cracking resistance.

The complicated spatial variation of the residual stress field depends on the elastic properties of grains, the grain size and the shape distribution. The residual stress across the grain boundary can be sufficiently large to initialise boundary microcracking. In elastic solids the stress σ_T is given by Blendel and Coble (1982):

$$\sigma_T = \beta\, E\, \Delta\alpha\, \Delta T \tag{1}$$

where β is a coefficient dependent on the shape and the grain orientation ($\beta \in < 0.5, +0.5 >$)[1], E is Young's modulus, $\Delta\alpha$ is a difference in the single-crystal thermal expansion coefficients along the direction

considered, ΔT is a difference between the temperature T_c (at which the sample was stress-free) and the room temperature T_0. Value of $\Delta\alpha$ for alumina was found in the paper [2] and equals 0.9 E-6 K^{-1}.

Solution of the elastic body equilibrium problem, which is caused by thermal expansion orthotropy by finite elements method (FEM) leads to the solution of the body equilibrium equations with special materials model [7]. For the elastic materials the main matrix equation can be written as follows:

$$KU = P \tag{2}$$

where K is the stiffness matrix which depends on geometry and materials properties, U is the unknown nodal displacements vector and P is force loading vector. For the heating and cooling process the vector P is a function of thermal strains too. The strains depend on the temperature increment ΔT and thermal expansion coefficients, which show the phenomenon of orthotropy. Solution Eqn. 2 and calculation U vector allows us to calculate strains and then, using Hook's law, the body stress. The advantage of the FEM calculations presents the possibility of using the same finite elements mesh for any vector P (loading force which aggregates nodal forces, pressure and forces caused by temperature, etc.) and any boundary conditions. Finite elements method allows analysing of any real element of structure while taking into consideration real loads.

FEM MODELS OF POLYCRYSTALLINE ORTHOTROPIC CERAMICS

The calculations were made for a prism that was assumed to be an internal part of an „infinite" ceramic body, filling very small volume of the body. The body is an element of analysed ceramics structure and the prism is the volume containing a number of ceramic grains. The body can be a real element of any ceramic structure (macroscopic scale). The prism presents a finite volume of ceramic body in microscopic scale. The model contains cubic and polyhedral grains (Figure 1). It allows changing of the proportion between sizes of cubic and polyhedral grains in the model (Figure 2).

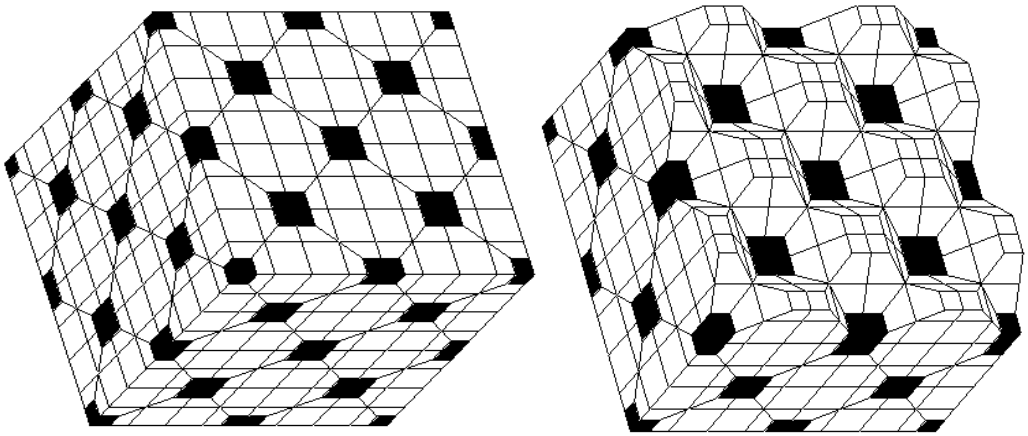

Figure 1: The model of cubes and polyhedrons

The grain size coefficient S was defined as a relation between current cubic grain size x and characteristic dimension of the finite element mesh X. The X value is constant for all of the models. For S=1 model contains only cubic grains. The other acceptable values of coefficient S vary from 0.3 to 0.7, to avoid computational errors resulting from excessive finite elements deformations. The set of grains labelled „A" begins in the corner of the model (Figures 1,2,3).

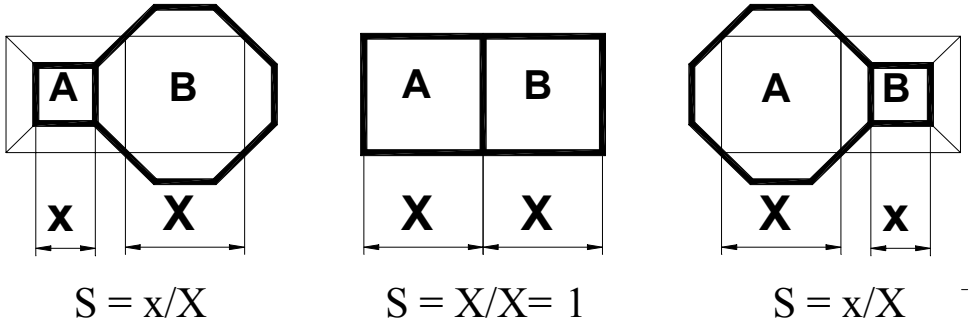

Figure 2: Definition of the grain size coefficient S=x/X

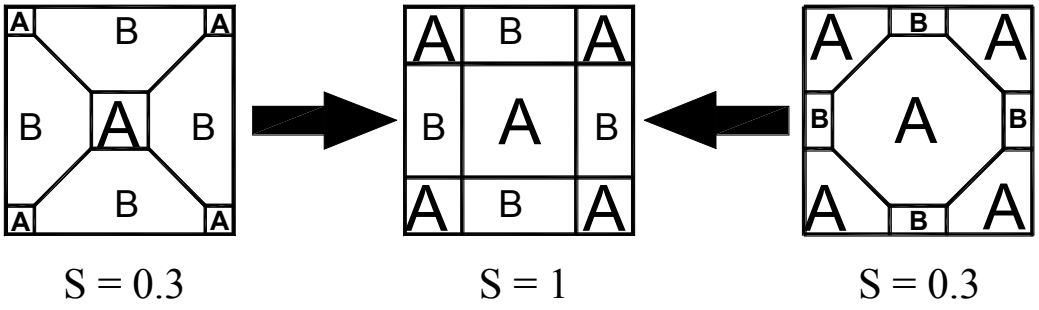

Figure 3: The unit of models may be obtained by changing size and shape of grains

For each grain the orthotropy direction c is chosen at random [6] from a set of possible axes. An exceptional requirement is verified during the randomising process. The directions of orthotropy must be different in the neighbouring grains. This requirement may be completed during the grain generation process by checking grains that had been defined earlier than the current grain (Figure 5a,b).

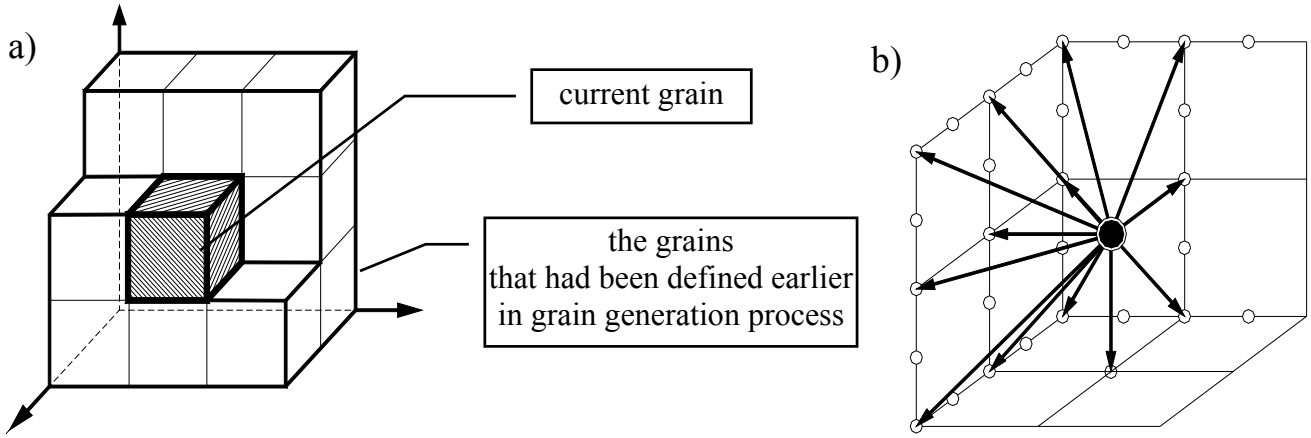

Figure 4: Scheme of grains generation and the set of possible directions

METHOD OF CALCULATIONS

A „two-steps" method was used for all the models. Firstly, it was assumed that the displacements of the prism boundaries were obtained from calculation for thermally loaded an isotropic element of ceramics structure. Secondly, it was assumed that the prism consists of ceramic grains. The grains were assumed to be thermally orthotropic. The calculations were made for the prism's boundary displacement from the first step and for the same thermal load. The calculations were made for the following values of parameters: Young's modulus E=380 GPa, Poisson's ratio ν=0.25, ΔT=1150 K, thermal expansion coefficients $\alpha_a=\alpha_b$=8.6E-6 K^{-1}, α_c=9.5E-6 K^{-1} (a, b, c – grain orthotropic axies), isotropic thermal expansion coefficient α = 8.9E-6 K^{-1}.

STATISTICAL POSTPROCESSING OF RESULTS

The distribution of each component of stress may be counted by summing the appropriate values calculated in integration points in the finite elements. The distribution may be obtained for the entire model, as well as for the cubic and polyhedral grains separately (Figures 5,6).

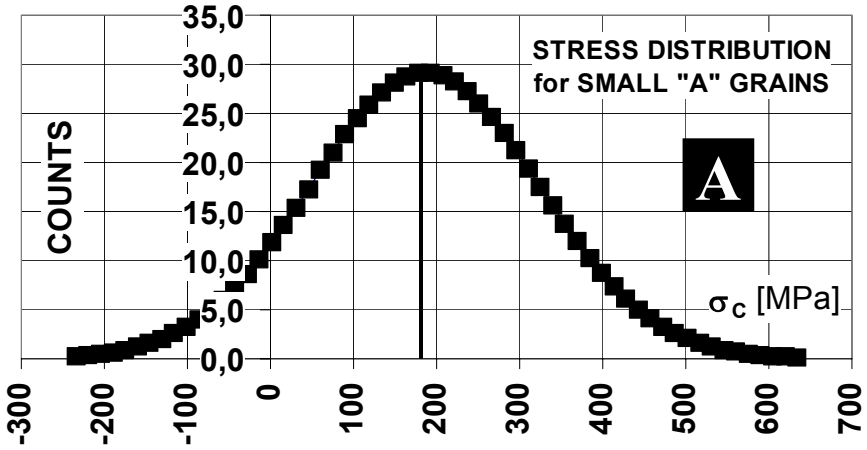

Figure 5: The σ_c distribution for small, cubic „A" grains, for the size coefficient S=0.3

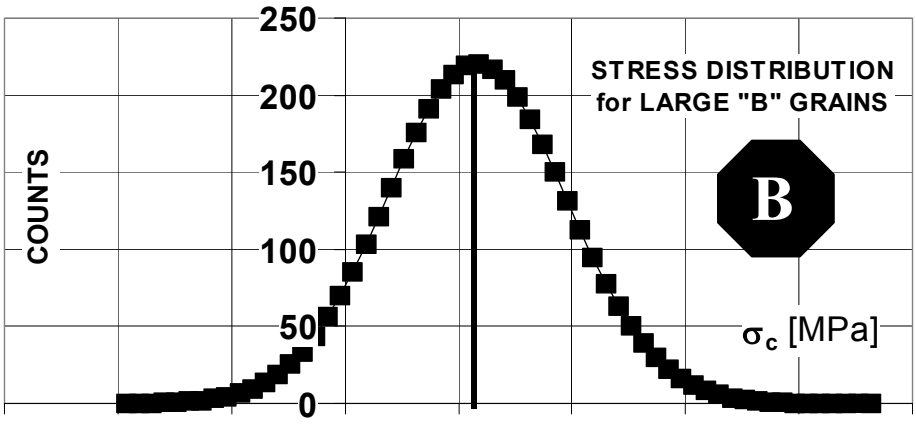

Figure 6: The σ_c distribution for large, polyhedral „B" grains, for the size coefficient S=0.3

Figure 7 shows the composition of σ_c average values (peak positions of stress distribution) obtained separately for „A" and „B" grains. They produce two separate curves. Each of them consists of two parts. Part A1 belongs to „A" grains of cubic shape and part A2 belongs to „A" grains of polyhedral shape. Adversely, part B1 belongs to polyhedral „B" grains and part B2 belongs to cubic „B" grains.
For example, part A1 shows that the σ_c value decreases from 186 MPa to 139 MPa when the grain size coefficient S enlarges from value of 0.3 to 0.7. For S=1 there are only cubic "A" and cubic „B" grains in the model with σ_c stress value of 133 MPa. Then, beyond this point, cubic „A" grains turns into polyhedral „A" grains and produce the curve A2.

An example of contour plot for σ_c stresses is presented below.

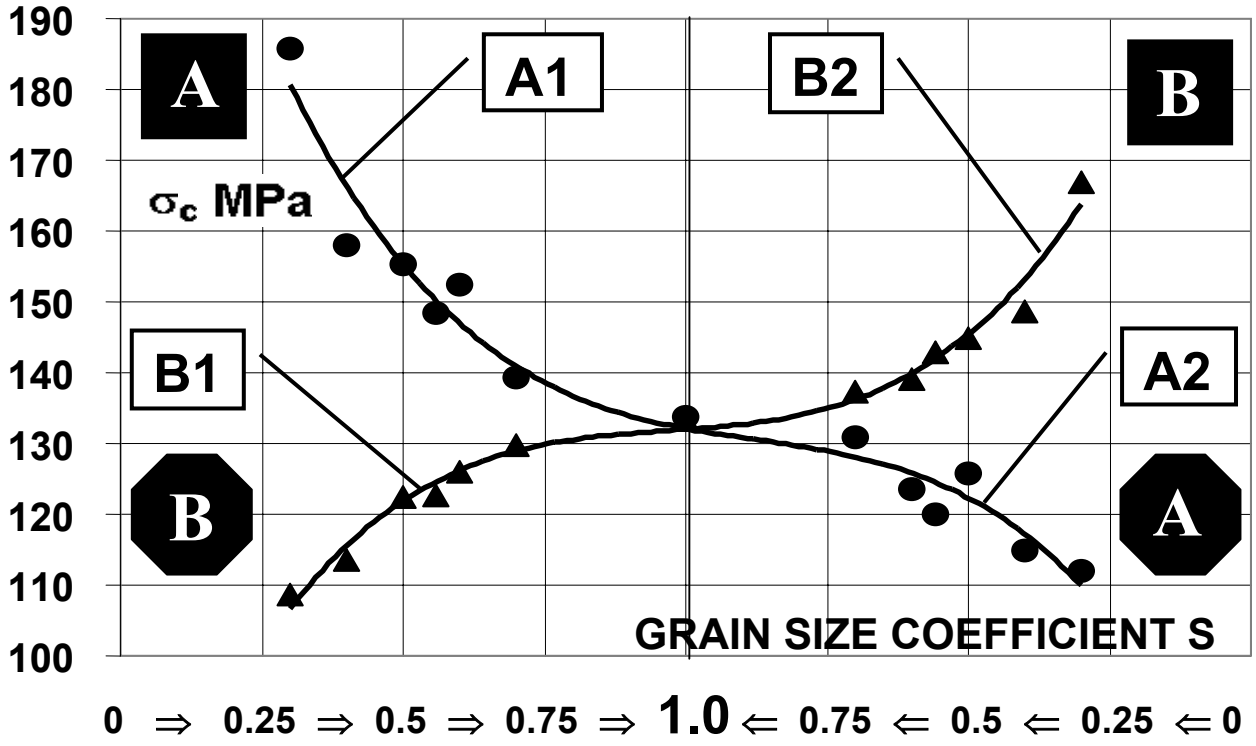

Figure 7: Composition of the σ_c average values that were obtained separately for „A" and „B" grains, for the unit of models with the same arrangement of ***c*** axes orientation, for various values of the grain size coefficient S

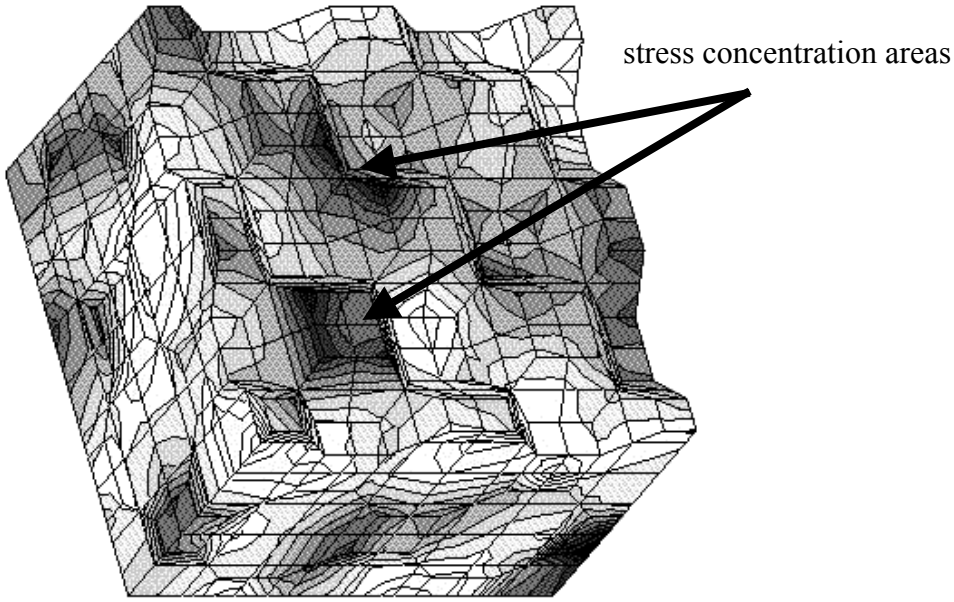

Figure 8: Example of contour plot for the values of σ_c, that is useful only for qualitative assessment of calculated stresses - it shows out the stress concentrations on external surfaces of grains

CONCLUSIONS

The proposed type of modelling of ceramic microstructure improved recently enables investigations of relative grain size influence on stress distribution, for neighbouring grains of different sizes grouped together in the same volume. The greater difference in size between neighbouring grains the higher stresses in small grains are observed. The model presented here may be used for investigations of ceramics (Al_2O_3) and ceramic composites (Al_2O_3 and ZrO_2) as well.

Using the statistic postprocessing of numerical results, the quantitative assessment of stresses in the modelled microstructure is possible [8]. The stress values calculated in integration points of finite elements are counted, to obtain stress distribution in the modelled volume of material. Then the peak position of the distribution is interpreted as the average stress value. This makes the numerical investigations similar to an experimental technique used for average residual stress measuring (the piezospectroscopic technique was enabled to verify numerical results).

The values of calculated average stresses are comparable with the results of our experiment [4] (the piezospectroscopic technique was enabled) and remain in a good agreement with those described in the works of other authors [1,3,5].

The results of calculations presented in the form of contour plots are useful for qualitative assessment of calculated stresses. They show that the significant part of internal energy in the modelled volume of microstructure is concentrated in the area close to the grain boundaries.

The advantage of numerical simulations is that the stress distribution may be counted separately for apportioned grains (e.g. of different size: small or large).

References

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