Modelling stress-strain state in oxide ceramics under thermal shock

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Abstract. Properties of ZrO$_2$-Al$_2$O$_3$ ceramic composites were studied in the framework of this research. The porous medium significantly affects the strength of the composite under thermal shock. In the areas near pores, concentrators emerge in a combined stress state with the maximum normal stresses under tension being equal to the compressing ones in absolute values and reaching 2.6 GPa (clusters of pores, 6% porosity) and 2.7 GPa (irregular distribution of pores, 12% porosity). High levels of stress lead to cracks in bridges between pores. The growth of porosity from 6% to 12% increases the number of dangerous zones.

1. Introduction
Thermal stability - an important functional property to materials, operating under frequent cyclic temperature changes. Some of the heat-resistant ceramic materials usually referred designed to work in conditions of thermal shock, high temperature gradients, as well as cyclical effects [1, 2, 3]. The questions of theoretical and experimental investigation of the thermal stability of the composite ceramic materials are relevant in the present. The objective of this research is to modeling stress-strain state in oxide ceramics under thermal shock.

2. Description of Model Parameters
The purpose of this work was to use conventional approaches of solid mechanics to evaluate the stress-strain state resulting from temperature distribution within the following oxide ceramic specimens under thermal shock with inclusions and porous structure (figure 1).

We show that it is possible to take into account experimental data on the microstructure of the Al$_2$O$_3$ – ZrO$_2$ nanocomposite specimens at hierarchical scale levels (nano, micro, meso, and macro) when creating model representative volumes of ceramic materials represented in the figure with and without porosity structure. Using the data on representativity of volumes from [4, 5], models were created representing structured representative volumes at mesoscopic level for mathematical simulation with due consideration of distribution of precipitate particles of ZrO in Al$_2$O$_3$ matrix in model a); presence of clusters of pores (6% porosity) in model b); and with due account for irregular distribution of pores (12% porosity) and precipitate particles of ZrO$_2$ (in model c). The dimensions of model specimens are 7.5 $\times$ 7.5 $\mu$m. Designations (a), (b) and (c) in figures hereinafter correspond to modeled meso-volumes depicted in figure 1.
Figure 1. Models of meso-volumes of oxide ceramics based on Al₂O₃ with precipitate particles of ZrO₂ (a); with due consideration of pore clusters (b); with due consideration of irregular distribution of pores and precipitate particles of ZrO₂(c).

Figure 2. Gridded model.
The figure 2 shows a gridded model. Geometric models of representative meso-volume elements are discretized by gridded models consisting of quadrilateral elements. There are approximately 7,000 elements on the grid. The choice of the grid density and dimensions of finite element was based on the results of grid convergence evaluation. The study also addressed a related thermomechanical problem to model thermal shock in ceramic composite. The problem was solved in two steps. First, we tackled the temperature problem where we had to determine the distribution of temperature fields in the material as a result of rapid cooling. Second, we used the results of the temperature problem to determine the stress-strain state of model specimens resulting from the thermal expansion of the material. The gridded model remained the same for both types of problems. The problem was solved as a two-dimensional one, i.e. the thickness of the model is much smaller than the other two dimensions. Such a statement allows analyzing the distribution of temperature and stress in the two-dimensional approximation.

The composite models under consideration have a grain structure and are similar in outside measurements, which can be idealized by the perimeter of computational domain ABCD shown on the scheme (figure 1). In the temperature problem, the computational domains are subjected to intense cooling by the side AB. We chose aluminum oxide Al$_2$O$_3$, as the matrix material and ZrO$_2$ as the inclusion material.

![Figure 3. Schematic representation of computational domain.](image)

In solving the temperature distribution problem in the computational domain, the system of linear algebraic equations corresponding to the grid comprised approx. 7,000 equations. The nonstationary heat conduction problem was solved by an implicit scheme [6].

For calculation we used the thermophysical material properties shown in Table 1.

| Table 1. Thermophysical material properties |
|---------------------------------------------|
|                | Al$_2$O$_3$ | ZrO$_2$ |
| $a$ $C$, J/(kg °C), | 1106        | 660     |
| $\rho$, kg/m$^3$ | 3800        | 6000    |
| $b$ $K_{xx}$, $K_{yy}$, W/(m °C) | 30          | 3       |

$^a$ $C$ is heat capacity, $\rho$ is density.
$^b$ $K_{xx}$, $K_{yy}$ are coefficients of heat conductivity along $x$ and $y$ axes.

3. Solution to the Heat Conductivity Problem
For the temperature field in the two-layer plate to be found by the finite element method [7, 8], a nonstationary heat conduction problem is solved for the domain ABCD. At the interface of the material differing in physical and mechanical characteristics, the thermal contact is perfect: the
temperatures and heat fluxes are equal [7]. The edges AC and BD are assigned the symmetry conditions:

$$\left. \frac{\partial T}{\partial x} \right|_{AC} = 0, \quad \left. \frac{\partial T}{\partial x} \right|_{BD} = 0.$$  \hspace{1cm} (1)

These conditions (called sometimes heat insulation conditions) mean that the introduced boundaries artificially narrow down the region under study and in a real situation the adjacent region has the same characteristics as the computational domain.

The edges AB and CD kept respectively at temperatures of 22 °C and 800 °C are assigned the Dirichlet conditions:

$$T|_{AB} = 22 \degree \mathrm{C}, \quad T|_{CD} = 800 \degree \mathrm{C}.$$  \hspace{1cm} (2)

At the point in time $t = 0$, the temperature over the entire domain ABCD is 800 °C:

$$T(x, y) = 800 \degree \mathrm{C}.$$  \hspace{1cm} (3)

In solving the problem by the finite element method, the heat conduction equation with boundary conditions (1) and (2) is reduced to minimization of the functional [6]:

$$\chi = \int_V 0.5 \left[ K_{xx} \left( \frac{\partial T}{\partial x} \right)^2 + K_{yy} \left( \frac{\partial T}{\partial y} \right)^2 + 2\lambda \frac{\partial T}{\partial t} T \right] dV,$$  \hspace{1cm} (4)

where $\lambda = c \rho$, $K_{xx}$, $K_{yy}$ are the thermal conductivities; $c$ is specific heat capacity; $\rho$ is the density, and $V$ is the domain volume.

The temperature field distributions in the material of the specimens are presented in figure 4.

![Temperature field distributions in model specimens.](image)

The distribution of temperature fields in computed areas is nonuniform due to different thermophysical characteristics of material of matrix and inclusions, presence of voids.

4. Analysis of Stress-Strain State

The next step makes use of the results from the temperature problem. As it has been established, intense heating of the heterogeneous plate gives rise to thermal stresses. The thermal stresses are estimated by solving the stress-strain state problem. It is assumed that at the contact boundary of the grains, the adhesion is perfect: the displacements and stresses are equal. The stress-strain state problem
is solved using the finite element method (FEM) [6]. In terms of strength estimation, if there is a temperature with large gradient under thermal shock, this indicates a dangerous state.

The potential energy of an elastic solid acted by surface forces $P_x$, $P_y$, and $P_z$ with initial strain $\varepsilon_0$ is [5]:

$$
\Pi = \sum_e \int \frac{1}{2} \{U\}^T [B^{(e)}]^T [D^{(e)}] [B^{(e)}] \{U\} dV - \sum_e \int \frac{1}{2} \{U\}^T [B^{(e)}]^T [D^{(e)}] [B^{(e)}] \{\varepsilon_0^{(e)}\} dV
$$

$$
- \sum_{e} \sum_{S^{(e)}} \frac{1}{2} \{U\}^T [N^{(e)}]^T \left[ \begin{array}{c}
P_x^e \\
P_y^e \\
P_z^e
\end{array} \right] dS,
$$

where $\{U\}$ is the displacement vector; $[B^{(e)}]$ is the strain-displacement matrix containing derivatives of shape function; $[D^{(e)}]$ is the elasticity matrix; $\{\varepsilon_0\}$ is the initial strain vector; $[N^{(e)}]$ is the matrix containing shape functions; $P_x$, $P_y$, $P_z$ are the surface load intensities along the axes; $S^{(e)}$ is the area of elements acted by the surface load; $V$ and $S$ are the volume and area of the elastic solid.

Resulting equations of the finite element method are derived from minimization conditions of the total potential energy functional $\Pi$ of the mechanical system:

$$
\frac{\partial \Pi}{\partial \{U\}} = 0
$$

The minimization of the functional $\Pi$ gives the system of linear algebraic equations:

$$
[K] \{U\} = \{F\}
$$

where $[K]$ is the global stiffness matrix of the mechanical system and $\{F\}$ is the force vector.

The global stiffness matrix of the finite element grid is equal to the sum of stiffness matrices of individual elements. The global force vector $\{F\}$ is equal to the sum of force vectors of individual elements $\{f^{(e)}\}$:

$$
\{F\} = \sum_e \{f^{(e)}\}
$$

The force vector of a single finite element with surface forces $P_x$, $P_y$, $P_z$ and initial strains is written in the form:

$$
\{f^{(e)}\} = \int \{B^{(e)}\}^T [D^{(e)}] \{\varepsilon_0^{(e)}\} dV + \int_{S^{(e)}} \{N^{(e)}\}^T \left[ \begin{array}{c}
P_x^e \\
P_y^e \\
P_z^e
\end{array} \right] dS
$$

The initial strain vector for the plane stress state is equal to

$$
\{\varepsilon_0\} = \alpha \Delta T \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}
$$

where $\alpha$ is thermal expansion coefficient ($1/°C$); $\Delta T$ is the temperature difference of a single finite element ($°C$).
For the plane stress state, the integral related to thermal expansion (initial strain) is equal to

\[
\int \{B^{(e)}\}^T[D^{(e)}]\{\varepsilon_0^{(e)}\}dV = \frac{Ea_\alpha\Delta T}{2(1-\nu)} \begin{pmatrix} b_i \\ c_i \end{pmatrix}, \quad \begin{pmatrix} b_j \\ c_j \end{pmatrix}, \quad \begin{pmatrix} b_k \\ c_k \end{pmatrix}
\]

where \(E\) is Young's module (MPA); \(\nu\) is Poisson's ratio; \(a_i\) is the thickness of an element. The coefficients \(b_j, c_j, b_k, c_k\) are derived by circular substitution.

For the plane stress state, the initial strain vector \(\{\varepsilon_0\}\) and the elasticity matrix \([D^{(e)}]\) change [6]. The integral related to thermal expansion for plane strain is equal to

\[
\int \{B^{(e)}\}^T[D^{(e)}]\{\varepsilon_0^{(e)}\}dV = \frac{Ea_\alpha\Delta T}{2(1-2\nu)} \begin{pmatrix} b_i \\ c_i \end{pmatrix}, \quad \begin{pmatrix} b_j \\ c_j \end{pmatrix}, \quad \begin{pmatrix} b_k \\ c_k \end{pmatrix}
\]

Like in the previous calculation, the grid contained about 7,000 finite elements; the number of algebraic equations whose solutions give the displacement vector was 7,000.

The result of problem solving was displacement, strain and stress fields in the cross-section of the plate ABCD. In solving the plane elastic problem, symmetry conditions were specified in the domain ABCD. As with the thermophysical problem, the introduced boundaries artificially narrow down the dimensions of the area to be analyzed, while in a real case the adjacent area is assumed to have the same characteristics as the calculated one.

At the edge CD, the displacement \(V\) along the axis \(y\) is equal to zero, i.e.

\(V \mid_{CD} = 0\)

(13)

on the lines AC and BD, the displacement \(U\) along the axis \(x\) is equal to zero, i.e.

\(U \mid_{AC} = 0, \quad U \mid_{BD} = 0\).

(14)

The stress-strain state was calculated with the physical and mechanical characteristics of the materials and precipitate inclusions presented in the table.

**Table 2. Physical and mechanical characteristics of materials.**

|                  | \(\text{Al}_2\text{O}_3\) | \(\text{ZrO}_2\) |
|------------------|-----------------------------|------------------|
| \(E, \text{GPa}\) | 380                         | 210              |
| \(G, \text{MPa}\) | 153                         | 84               |
| \(\nu\)          | 0.35                        | 0.35             |
| \(\alpha, 10^6/\degree\text{C}\) | 9.0                         | 0.11             |
Figure 5 and 6 show surfaces illustrating the distributions of normal stresses $\sigma_y$ of the stress tensor and $\sigma_{11}$ of the tensor of main stresses, caused by nonuniform distribution of temperature along the plate thickness, depicted in Fig. 4.

The difference between thermophysical and physicomechanical characteristics of the material of inclusions and matrix as well as porosity and the temperature gradient together affect the stress-strain state of the composite.

The pore-free medium with inclusions suffers the occurrence of negligible tensile strains in the area of the inclusions equal to 588 MPa. The normal stress in the compression area is 298 MPa. Calculations demonstrate that tensile stresses introduce the maximum contribution to stress-strain state of the considered non-porous composite with the clustered distribution of inclusions. Under such conditions of temperature distribution in the considered meso-volume, the composite sustains thermal shock without fracture.

The porous medium appreciably affects the strength of the composite under thermal shock. The consideration of porous medium results in a combined stress state. In the areas near pores, concentrators emerge with maximum normal stresses that under tension are equal to compressing ones in absolute values and reach 2.6 GPa (clusters of pores, 6% porosity) and 2.7 GPa (irregular distribution of pores, 12% porosity). High levels of stress lead to cracks in bridges between pores. Increased porosity from 6% to 12% lead to an increase in the number of dangerous zones.

Figure 5. Distribution of normal temperature stresses $\sigma_y$ in model volumes.
5. Conclusion

The following major factors were revealed as a result of solution of coupled thermomechanical problems on stress-strain state under thermal shock in representative volumes of ceramic composites having Al$_2$O$_3$ matrix with precipitate particles of ZrO$_2$ and pores:

- Distribution of temperature in material is nonuniform; the distribution of temperature fields is appreciably distorted by inclusions and pores with thermophysical characteristics that differ from those of matrix material;

- The pore-free medium with inclusions suffers the occurrence of negligible tensile strains (less than 600 MPa) in the area of the inclusions. The composite sustains thermal shock without fracture.

- The porous medium significantly affects the strength of the composite under thermal shock; in the areas near pores, concentrators emerge in a combined stress state with the maximum normal stresses under tension being equal to the compressing ones in absolute values and reaching 2.6 GPa (clusters of pores, 6% porosity) and 2.7 GPa (irregular distribution of pores, 12% porosity). High levels of stress lead to cracks in bridges between pores. The growth of porosity from 6% to 12% increases the number of dangerous zones.

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