The Modeling of Mechanical Properties of Dolomite Ceramics

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Abstract. This publication presents the model and the modeling results of dolomite ceramics deformation under uniaxial load with respect to the composite structure of dolomite ceramics. The main modelling objective was to investigate the dependence of mechanical properties of dolomite ceramics on the mechanical properties and volume proportions of its components – clay and dolomite, assuming the composite structure of dolomite ceramics. The dependencies of theoretical integral elasticity module and local stress concentration coefficients on elastic moduli and volume proportions of were investigated by means of mathematical experiment, and presented as curves, thus making conclusions about the impact of mechanical properties and volume proportions of components on the expected elastic module and tension/compression strength of dolomite ceramics.

Keywords: dolomite ceramics, clay, dolomite, elasticity modulus, strength, stress concentration, mathematical modeling.

I. INTRODUCTION

Clay is one of the most popular materials in Latvia since the ancient times. It is used in pottery as construction and insulation material. From environmental and economic perspectives, clay bricks, roof tiles, pavers, plaster plates and other products are valuable, healthy and efficient construction materials with excellent properties.

The potential amount of clay deposits in Latvia is about 211 mil. m³ [1]. It is the third most common type of raw materials by volume after gravel and limestone.

Traditionally, ceramic raw materials are plastic clay, lea agents, fluxes and burning-out additives. Clay makes up the major part of raw materials.

Fluxes are substances with high melting temperature, which during firing produce a low melting-temperature eutectic mixture with clay minerals. The amount of flux added to common ceramics varies in the range 0–20%; firing temperature reaches 1000° C and more. Ground limestone, chalk or marble are used as fluxes. It is possible to use dolomite CaMg (CO₃)₂ as flux material.

For the effective use of local raw materials and for the purpose of energy saving, it is important to develop ceramic materials with the lowest possible firing temperature, which are produced from cheap raw materials, and possess mechanical properties that are the same or even better than those of traditional materials. The research concerning the development of such materials is being carried out within the framework of ERAF Project “Elaboration of Innovative Low Temperature Composite Materials from Local Mineral Raw Materials” (No. 2010/0244/2DP/2.1.1.1.0/10/APIA/VIAA/152) by using such raw materials as local dolomite processing residues – dolomite flour (dolomite from JSC “Saulkalne”, quarry Kranciems) and clay from Liepa deposit [2]. Taking into account that in the experimental samples of dolomite-clay composite material the proportion of dolomite is significantly higher than in traditional ceramic materials, new ceramic material has been named “Dolomite ceramics”.

II. MATERIAL STRUCTURE, CALCULATION MODEL AND MAIN ASSUMPTIONS

For the qualitative assessment of material structure, the micro cuts of samples of dolomite ceramics were prepared. Typical cut surface pictures under a digital microscope "Keyence VHX-300" are presented in Fig. 1.

As it can be seen (Fig. 1), the dolomite particles are distributed relatively uniformly in material volume. The size of particles varies in the range from 60 to 90 µ, whereby the size of conglomerate particles reaches approx. 200 µ. The calculation model, mentioned below, is based on the assumption of uniform distribution of the same size particles.

The calculation model of dolomite ceramics structure assumes that the material consists of homogenous clay matrix, in which there are spherical dolomite particles of equal size that are uniformly distributed. The volume centred cubic structure is assumed (Fig. 2). This type of structure is known as one of main particle arrangements [4, 5].

The volume centred cubic arrangement allows for a more dense maximal packing of dolomite particles compared to a simple cubic arrangement (Fig. 2a). The relative volume proportion of particles/(repeating element) can be expressed by means of volume factor ψ. Thus, the maximal possible volume factor for a simple cubic arrangement (Fig. 2a) is as follows:

\[ \psi_{\text{max}} = \frac{\pi}{6} \]

However, the maximal possible volume factor for volume centred cubic arrangement (Fig. 2b) is as follows:

\[ \psi_{\text{max}} = \frac{\pi \sqrt{3}}{8} \]
Regarding the deformation of composite material model, it is assumed that the direction of linear tension/compression loading and main linear deformation direction coincide with model mesh edge direction \( X \). Taking into account the model particle arrangement symmetry, it is possible to cut out the repeating element (Fig. 3a) with face remaining plane and angles between faces remaining unchanged in the deformed state.

The repeating element (Fig. 3a) is assumed to be made of prismatic elements, oriented parallel to main deformation direction \( X \) (Fig. 3b). Each prism of initial length (in non-deformed state) \( L \) consists of matrix material A of length

\[
L_{Ai} = X_{2i} - X_{1i}
\]

and particle material B of length

\[
L_{Bi} = L - L_{Ai}
\]

Coordinates \( X_{1i} \) and \( X_{2i} \) (prism crossing points with spheres) depend on considered prism coordinates \( Z_i \) and \( Y_i \) in a repeating element (Fig. 3a).

\[
X_{1i} = \begin{cases} 
\sqrt{R^2 - Y_i^2 - Z_i^2} & \text{for } (R^2 - Y_i^2 - Z_i^2) \geq 0 \\
0 & \text{for } (R^2 - Y_i^2 - Z_i^2) < 0
\end{cases}
\]

(3)

\[
X_{2i} = \begin{cases} 
L - \sqrt{R^2 - (Y_i - L)^2 - (Z_i - L)^2} & \text{for } (R^2 - (Y_i - L)^2 - (Z_i - L)^2) \geq 0 \\
L - \sqrt{R^2 - (Y_i - L)^2 - (Z_i - L)^2} & \text{for } (R^2 - (Y_i - L)^2 - (Z_i - L)^2) < 0
\end{cases}
\]

(4)

In case of axial tension in \( X \) direction the elongation of all prisms is equal to \( \Delta L \):

\[
\Delta L = \Delta L_A + \Delta L_B
\]

(5)

where \( \Delta L_A \) and \( \Delta L_B \) are elongations of each prism matrix and particle materials respectively.
On the other hand, according to Hooke's law:

$$\Delta L = \sigma \frac{L}{E}$$  \hspace{1cm} (6)

where $\sigma$ – the normal stress in prism;

$E$ – the modulus of elasticity of prism.

Assuming that the deformed prisms do not interact with each other through their side surfaces (neglecting the shear effect), the normal stress $\sigma$ can be taken as constant over the length of each prism. In such a case:

$$\Delta L_A = \sigma \frac{L_A}{E_A}; \quad \Delta L_B = \sigma \frac{L_B}{E_B}$$  \hspace{1cm} (7)

where $E_A$ and $E_B$ are moduli of elasticity of matrix and particle materials respectively.

Equations (5–7) result in the formula for the modulus of elasticity of prism number $i$:

$$E_i = \frac{L}{\frac{L_{Ai}}{E_A} + \frac{L_{Bi}}{E_B}}$$  \hspace{1cm} (8)

In mechanics, the formula given above is known as the modulus of elasticity of “serially connected elements”.

Assuming the unitary mean deformation, the normal stress in prism number $i$ is as follows:

$$\sigma_i = E_i$$  \hspace{1cm} (9)

Considering that the integral force acting onto repeating element is equal to sum of forces on all prisms, the modulus of elasticity of repeating element is given by the following formula:

$$E = \frac{\Delta S}{S} \sum_{i=1}^{n} E_i = \frac{1}{n} \sum_{i=1}^{n} E_i$$  \hspace{1cm} (10)

where $S$ – the cross-section surface of repeating element (perpendicular to $X$);

$\Delta S$ – the cross-section surface of one prism;

$n$ – the number of prisms.
In case of unitary deformation, the mean stress in repeating element is given by the following formula:

$$\sigma_m = \frac{E}{n \cdot \sum E_i}$$

(11)

From (9-11) it is possible to calculate the stress concentration coefficient or the relation of stress $$\sigma_i$$ to mean stress $$\sigma_m$$:

$$k_i = \frac{\sigma_i}{\sigma_m} = \frac{n \cdot E_i}{\sum E_i}$$

(12)

The maximum value of this coefficient gives the approximate assessment of strength reduction of composite material in relation to the strength of the weakest component, because initial damage in an ideal case can be expected at the points of maximal stress concentration. In regular structures such local damage is likely to cause the cascading total damage [5].

The presented simplified model may be considered an individual case of “bundle model” [6], being used in fracture mechanics. Similar model, where the repeating element of composite structure is assumed to consist of finite thickness layers, is used in [7] to calculate the transversal modulus and stress concentration in unidirectionally reinforced plastic.

According to this model, each prism (Fig. 3b) can be considered a finite element or part of “bundle”. In both the undeformed and deformed state, prism ends are joined together, staying in one plane, perpendicular to a main deformation direction. Such geometrical behaviour of the model is due to the model symmetry, where the side faces of repeating element (Fig 3a) remain plane during deformation.

There is no shear or frictional interaction between individual prisms; - this is the main assumption for a simplified model.

Modulus of elasticity E (Eq.10) and stress concentration coefficient $$k_i$$ (Eq. 12) are the main factors, characterizing the calculation model. They depend on the moduli of elasticity of component materials $$E_A$$ and $$E_B$$ and volume factor $$\psi$$ (relation of particle material volume to entire volume), connected to particle radius R:

$$\psi = \frac{\pi \cdot R^3}{3L^3}$$

(13)

Such a model can appear to be very simplified: the same size spherical particles, regularly distributed in volume, neglecting the normal stress distribution along the prisms of repeating element, etc. On the other hand, it is reasonable to assume, that the analysis of such a model gives the basic assessment of dependencies of maximal stress concentration and E-modulus on E-moduli and volume proportions of component materials.

III. MODELLING ALGORITHM

Algorithm is based upon equations (3-13). It was programmed and implemented as MS EXCEL macros. The algorithm performs the calculation of the modulus of elasticity E and stress in each prism. The maximum stress value

$$\sigma_{i_{\text{max}}}$$

is taken into account by calculating the maximum concentration coefficient $$k_{i_{\text{max}}}$$ according to Eq. (12). Input values are the moduli of elasticity of component materials $$E_A$$ and $$E_B$$, volume factor $$\psi$$ and number of prisms n in the repeating element.

The relative volume factor $$\lambda$$ was used, which was calculated as a relation of volume factor $$\psi$$ to its maximal value (Eq. 2):

$$\lambda = \frac{\psi}{\psi_{\text{max}}} = 1,54 \cdot \frac{R^3}{L^3}$$

(14)

The factor $$\lambda$$ varies from 0 to 1, and, according to (14):

$$R = L \cdot \frac{\sqrt[3]{1,54}}{\sqrt[3]{2}}$$

(15)

The test calculations were performed to assess the model discretisation rate, sufficient for stable results. Discretisation assumes the equal prism edge length $$\Delta Y$$ and $$\Delta Z$$ along Y and Z axes respectively (see Fig. 3). When $$n > 1600$$, for all possible $$\lambda$$ values, the calculation results (E and k), by doubling a number of prisms n, vary by less than by 1%. Taking this into account, further calculations were made for $$n=1600$$ ($$\Delta Y = \Delta Z = L/40$$).

Fig. 4 and Fig. 5 present the main modelling results – the modulus of elasticity E relative to the matrix modulus $$E_A$$ and the maximal stress concentration coefficient $$k_{i_{\text{max}}}$$ as functions of $$\lambda$$ by different values of relative modulus e (Eq. 16)

$$e = \frac{E_B}{E_A}$$

(16)
IV. RESULT ANALYSIS

The main modeling results are shown as curves in Fig. 4 and Fig. 5. These curves were obtained for a broad spectrum of model component material properties, by changing volume factor \( \lambda \) from 0.1 to 1 and relative elasticity modulus \( e \) from 0.2 to 4. On the other hand, literature data [2, 8-11] regarding the mechanical properties of clay and limestone, shows a significant variation in numerical values. The possible reasons for such variations are as follows:

- chemical composition differences (different extraction sites);
- changes in mechanical properties during firing [2];
• changing in mechanical properties due to hydration (limestone, after firing) [2,11];

The significant increase in maximal stress concentration \( k_{\text{max}} \) along with \( \lambda \) takes place in cases of bigger difference between moduli of elasticity of component materials. The highest \( k_{\text{max}} \) values were reached, when the modulus of elasticity of particle material was less than that of matrix material (curves \( e=0.4; e=0.2 \) in Fig. 5).

The correlation between modelling results and experimental results of strength dependence of dolomite ceramics on volume factor has been observed. The curves “\( e=2 \)” and “\( e=4 \)” (Fig. 5) have the minimum for \( \lambda = 0.8 \), which corresponds to the model material strength maximum. Such strength maxima for the same \( \lambda \) values can be observed in measurement results [10] (Fig. 1).

V. CONCLUSIONS

The material elasticity modulus \( E \) is integral factor, which explains its nearly linear dependence on volume factor \( \lambda \) (curves in Fig. 4).

For the effective use of component strength it is important to have components with possibly near values of moduli of elasticity, as well as the modulus of elasticity of particle material must not be less than that of matrix material.

The relation between the moduli of elasticity of component material significantly influences the strength of composite material (dolomite ceramics). It is important to investigate how the different chemical and physical processes influence the elastic properties of mineral materials (clay, dolomite).

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