The study of the influence of the parameters of the porosity of the medium on the effective modulus of elasticity

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Abstract. On the basis of the analysis of correlation characteristics of locally-elastic properties of modeling material the task of definition of locally-representative volume at different parameters of porosity is solved. For the analysis of dispersity of pores modeling cellular structures with volume content of 55 % and bimodal system of pores were considered. There were selected accidentally the limits of with representative volume 300 points in which local elastic properties were investigated. For definition of these properties each point on mesoscopical representative volume (MRV) level is presented by a small fragment of modeling frame of a porous media, MRV with characteristic for it geometry of frame of pores. Calculation of elastic properties of each such MRV was carried out by a method of final elements with use of the equipment of calculation of parameters tensely-strained state at mesolevel and their data smoothing. It is revealed that the ratio between the maintenance of large and small pores in dispersible-porous medium plays an important role. The dependence of an effective elastic module on a share of a time of large pores is set.

1. Introduction

The extensive use of porous materials, the development of new technologies for their production and the emergence of various types of these materials determine the development of methods for properties and mechanical behavior prediction during manufacturing and maintenance. The creation of appropriate techniques and reliable estimate of physical-mechanical properties, e.g. elastic, causes not only time and money cost reduction during the product design, but also estimation of efficiency and operational reliability of structural elements of these materials.

Fragile porous materials are often used in engineering, machinery and equipment. Sintered ceramics based on nanocrystalline metal oxides (in particular, aluminum and zirconium) is one of the instances of this class. Printed circuit boards and substrates of porous ceramics have high thermal conductivity and thermal expansion coefficient, close to the characteristics of the main semiconductor materials of electronics. In addition they have good electrical performance and tightness. Due to the large variety of technological modes of ceramics synthesis in its structure, there are pores of various sizes. The pore size distribution function of this material usually has several maxima. Moreover, the number of pores corresponding to each maximum of the distribution function may differ for each of the total porosity values, and it itself may vary within wide limits. In this aspect, ceramics is no longer just a porous body, but a certain structure which mechanical behavior and properties are determined by the indicated structure parameters. In practice, it is the combination of the parameters of the pore structure and the mechanical properties of the material that largely determines the area of its functional application.
Taking it into consideration it seems relevant and necessary to know the dependence of the properties of porous materials (and ceramics, in particular) on the specified parameters of the pore structure in the entire range of changes in their values.

To determine the considered characteristics (properties) it is necessary to be able to find their values at arbitrary points of the environment. These values and, accordingly, properties can be called local.

The local values of elastic moduli characterize the reaction of a certain volume of a porous material to external loads. The nature of this reaction largely depends on the size of the examined volume. Consequently, to solve the problem of determining local properties correctly, one needs to know the conditions for choosing a certain characteristic volume of a porous material, which would make it possible to determine the influence on the formation of its mechanical properties of such factors as the mechanical interaction of material components, the type of elementary deformation mechanisms, the volume content of structure elements etc.

Local representativeness is understood to mean that in determining the local properties of a material, only such structural elements are taken into account that make the greatest contribution to the formation of properties in the vicinity of a particular selected point. Evaluation of the contribution to the formation of mechanical properties of more and more distant elements of the material structure allows us to determine this volume. For materials with a random structure, these reliable estimates can only be obtained using the methods of statistical mechanics.

Taking into account aforementioned facts the goal of the work is to study the effect of porosity parameters on the effective modulus of elasticity.

2. Determination of the size of a locally mesoscopical representative volume (MRV) of a porous material

As noted in [1], many porous materials are characterized by the presence of bimodal porosity, while the pore size, which constitute the “large” fraction, is substantially larger than the pore sizes of the “small” fraction. In this regard, to conduct numerical modeling, we constructed geometric models of porous materials with different volume ratios of the “large” and “small” fractions, in which the ratio between the pore sizes of both fractions is assumed to be 8/1, which is quite typical for such materials. To analyze the dispersion of pores, model porous structures with a volume content of $C = 55\%$ and a bimodal pore system were considered. The presence of this porosity system in materials such as porous ceramics is noted in [2, 3]. The ratio of the diameters of small and large pores of 8 to 1 was taken for the model material.

Model materials were divided into four types (Table 1) based on the volume ratio between small ($C_d$) and large ($C_D$) pores.

| Type of model material | Volumetric content of pores, % |   |
|------------------------|-------------------------------|---|
|                        | $C_D$ | $C_d$ |
| 1                      | 80    | 20    |
| 2                      | 60    | 40    |
| 3                      | 40    | 60    |
| 4                      | 20    | 80    |

As an example, we take the model of porous material structure of type 1 with given volume ratios of pores in size. Volume, each side of which was 25 times the diameter of large pores, was considered
as representative. This size is considered sufficient to ensure the geometric representativeness of the model.

![Figure 1. Model of representative volume of porous material with a volume content of small ($C_r=20\%$) and large ($C_r=80\%$) pores.](image)

The elastic moduli of the pores $E_i=0.1$ GPa [4] and the matrix $E_m=40$ GPa, Poisson’s ratios of inclusions $\nu_i=0.2$, and the matrix $\nu_m=0.22$ were chosen as the values of the mechanical characteristics of the components. $N=300$ points were randomly selected within a representative volume at which local elastic properties were studied. To determine these properties, each point at the mesoscopic level is represented by a small fragment of the porous medium model structure and the MRV with its characteristic pore geometry. The calculation of the elastic properties of each MRV was carried out by the finite element method [5, 6] using the technique of calculating the parameters of the stress-strain state at the meso-level and their averaging [7].

In order to determine the size of locally representative volume of a simulated porous material, a sequence of paired samples of mesoscale was considered in accordance with the proposed method in [8]. The sizes of $L/d$ volumes (Figure 3) in this case varied from 0.8 to 4 in increments of 0.8, from 4 to 12 in increments of 2. Volume size of 24 was chosen due to evolved dependence.

In order to estimate the elastic properties of each volume, numerical simulation of its mechanical behavior under uniaxial loading was performed. The components of the stress and strain tensors found as a result of the simulation were used to calculate the effective value of the volume elasticity modulus:

$$E_{eff} = \frac{\overline{\sigma}_y}{\overline{\epsilon}_y},$$

where

$$\overline{\sigma}_y = \frac{1}{V_y} \int \sigma_y dV; \quad \overline{\epsilon}_y = \frac{1}{V_y} \int \epsilon_y dV,$$

and the index $y$ corresponds to the direction of loading.
The estimation of the locally representative volume of the porous material is based on the analysis of the dependence of the correlation function $R$ on the simulated volume $L_f$.

$$R_{E_1E_{||}} = E_1E_{||} = \int_{-\infty}^{\infty} E_1E_{||} f(E_1E_{||})dE_1dE_{||},$$

(3)

where $f(E_1E_{||})$ is the two-point distribution density of the local values of the elastic modulus for some value of the MRV.

The results are presented in Figure 2. The numbers of the curves in the plot correspond to the data given in Table 1.

![Figure 2](image)

**Figure 2.** Dependence of the correlation function $R$ on the size of the simulated volume $L_f/d$.

The tendency of the correlation function $R$ to unifunction [9, 10] is a sign of the local representativeness of the corresponding volumes. Thus, according to the results of the conducted simulation, it can be assumed that the volume not less than $L_f/d=24$ can be chosen as locally representative.

![Figure 3](image)

**Figure 3.** Histogram of the distribution of local elastic moduli of a locally representative volume with a pore volume content of $C_d=20 \%$, $C_d=80 \%$. 
It can be clearly seen from the histogram that the distribution of local mesoscopic moduli of elasticity is asymmetric. The presence of asymmetry allows to use the Weibull law in order to study statistical characteristics at the mesolevel.

At the same time, Figure 4 shows that the approximations of this distribution by the Weibull and Gauss laws are close to each other. This may indicate the proximity of this sample to the normal distribution.

![Figure 4. Weibull and Gauss distribution density functions of average values of local elastic moduli.](image)

3. Determination of the effective moduli of elasticity of the porous medium

After determining the representative volume, the effective elastic moduli were calculated by averaging the local moduli at different volume pore ratios (Table 2) at the mesoscopic level.

| Type of model material | $C_d/C_d$ | $E_{eff}$, GPa |
|------------------------|-----------|----------------|
| 1                      | 80/20     | 2              |
| 2                      | 60/40     | 1.736          |
| 3                      | 40/60     | 1.439          |
| 4                      | 20/80     | 0.971          |

As can be seen from the presented data, an increase in the content of large pores in the material leads to an increase in the effective modulus of elasticity of the porous medium, which significantly decreased relative to the modulus of elasticity of the matrix, in particular for a model material of type 1 - by 20 times relative to the matrix, and for a material of type 4 - 40 times.
Figure 5. Dependence of the effective modulus of elasticity $E_{\text{eff}}$ on the volume content of large pores $C_D$.

From the Figure 5 it can be seen that with an increase in the volume content of large pores ($C_D$), the value of the effective modulus of elasticity and confidence intervals grows. This effect can be explained by the possibility of forming the skeleton structure of the matrix with a high content of large pores, as shown in Figure 6, where the dark areas correspond to the framework of the porous medium, and the light areas - to the pores.

The results indicate a significant effect of the dispersion of the pore structure on the effective modulus of elasticity of the porous medium.
Conclusion

Thus, the problem of the locally representative volume determination of a model porous material was solved based on the analysis of the locally elastic properties correlation. It was found that the ratio between the content of large and small pores plays an important role in the formation of the elastic properties of a dispersive-porous medium. The results of the study allow to suggest that an increase in the proportion of large pores leads to an increase in the effective modulus of elasticity, which can be explained by the formation of a pronounced framework structure of the medium.

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