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## Numerical Modeling of the Porosity Influence on the Elastic Properties of Sintered Materials

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### Abstract:

*The effect of structural porosity on the elastic properties of sintered materials was studied using the new multi-pore unit cell numerical model - MPUC. Comparison between proposed MPUC model and previously adopted two-phase unit cell - FCC numerical model as well as available experimental data in literature, was done by comparing obtained values for modulus of elasticity - E, shear modulus - G and Bulk modulus - K. Results obtained by proposed MPUC model are in excellent agreement with available experimental data in literature. It was confirmed that material porosity regarding pores' size (volume fraction) has noticeable influence on elastic properties of sintered material. Less porosity in the material microstructure generally leads to noticeable higher values of E, G and K. For fixed volume fraction, shape of pores has no significant influence on elastic characteristics.*

**Keywords:** Modulus of elasticity; Shear modulus; Bulk modulus; Porosity; Sintered materials.

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### 1. Introduction

For some ceramic fabrication techniques the precursor material is in the form of a powder. Subsequent to compaction or forming of these powder particles into the desired shape, pores or void spaces will exist between the powder particles. During the ensuing heat treatment, much of this porosity will be eliminated. However, it is often the case that this pore elimination process is incomplete and some residual porosity will remain. Any residual porosity will have a deleterious influence on both, the elastic properties and strength. For example, it has been experimentally observed that for sintered materials the magnitude of the modulus of elasticity - E decreases with volume fraction porosity.

On the other hand, the development and application of porous materials is motivated by the continuous demand for lightweight constructions with enhanced mechanical properties as well as for biocomposites used as bone replacement in implant surgery. Porous materials have been used in a wide range of applications in various engineering structures such as ceramics and bioceramics, porous shape memory alloys, foam-like structures and thermal spray deposits. Unfortunately, mechanical properties are degraded by the presence of porosity

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in sintered material [1]. Fact that porosity reduces the mechanical properties considerably is extremely important where sintered materials are used as structural materials. Porosity is a defect formed by interfacial reactions, which generally causes a decrease in the mechanical properties of structural material. In the metallographic studies, pores are classified into four types: round pores, long and broad pores, long and fissured pores, and small, fissured pores [2].

As it is well known, the microstructure has a significant impact on mechanical properties. The effects of clustering and interfacial debonding of particles on the mechanical properties of sintered materials were the topic of majority of the prior studies. Number of studies confirmed the fact that less porosity in the material microstructure leads to higher material stiffness and strength, while an irregular shape of pores strongly influences the material fracture toughness and strength [3-7]. But sometimes porosity is quite necessary e.g. in biomaterial implants for the regeneration of bone tissue. Recently, development of hydroxy-apatite related porous biocomposite structure for the applications to bone implants and tissue engineering has become increasingly important because interconnected porosity in the structure allows cell penetration and proper vascularization of the ingrown tissue [8]. Numbers of theoretical predictive models have been developed to correlate porosity shape and size and the effective elastic constants by assuming the porous material as a special case of a two-phase material in which the second phase consists of pores. A detailed summary of these methods could be found in Herrmann and Oshmyan [9] and Wang and Tseng [10].

In the past decade numerical modeling became a powerful tool for studying influence of microstructure on mechanical properties for different types of materials. In the unit cell approach random distribution of pores is idealized by periodically distributed pores which are represented by a periodic repeating cell. The unit cell approach requires relatively little computational efforts in comparison to simulations of real structures and allows to study the effect of the mutual arrangement of phases in composite [11, 12] or cellular materials [13]. In this study, address is on the isolated porosities and their influence on modulus of elasticity, shear modulus and Poisson's ratio of sintered materials by using MPUC model. A face-centered-cubic (FCC) finite element (FE) unit cell model which was previously designed to evaluate the compressive stiffness and strength of biocomposite material for a range of porosity volume fractions [14] is used here for comparison purposes.

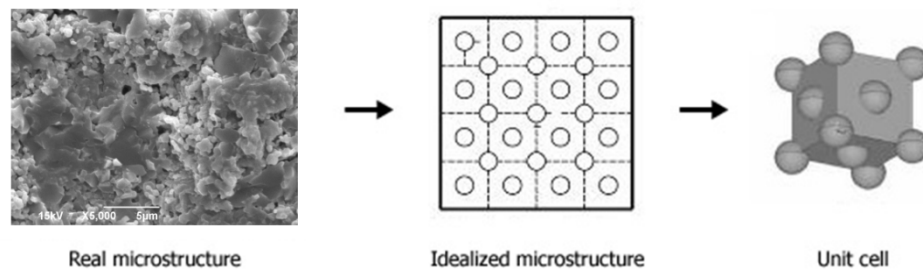
## 2. Materials and Experimental Procedures

### 2.1 Modeling procedure

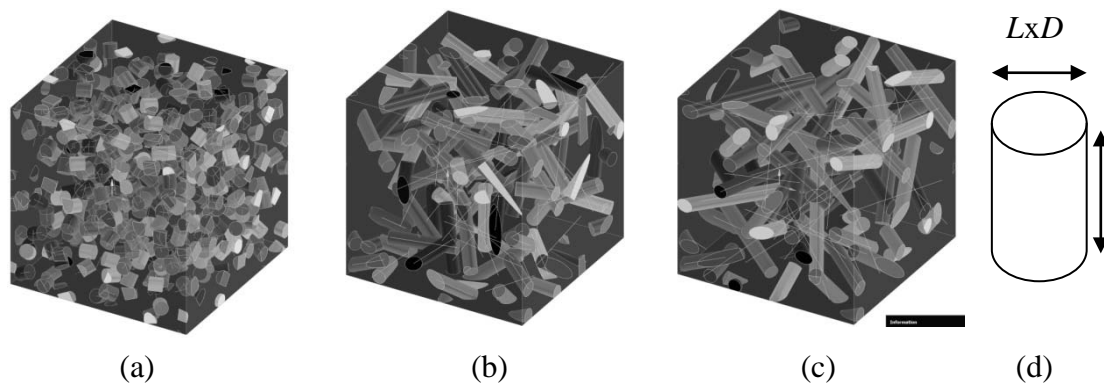
Typical microstructure of sintered material, after sintering process, usually leads to a denser microstructure, with closed pores and parts of well sintered grains as presented at Fig. 1 (SEM micrograph of sintered alumina at 1400 °C [3]). To fully simulate such a microstructure, a three-dimensional (3D) model of a random distribution of pores shape and size is required. The present study aims at carrying out a comparative evaluation of newly developed three-dimensional (3D) multi-pore numerical model (MPUC) versus two-phase unit cell (FCC) models which were used for predicting porous material elastic constants  $E$ ,  $G$  and  $K$ . In this study, distribution of pores is idealized by random distribution and orientation of approx. from 30 to 150 pores of the same size which are represented here by MPUC model. The irregular shape of porosity appearing in real microstructure, is idealized as cylinder geometry shape (Fig. 2 (d)) with randomly chosen orientation, while intersecting of cylinders is not allowed, as shown on Fig. 2 (a,b,c). Aspect ratio, length to diameter ratio -  $L/D$ , were chosen to be 1, 2, 5 and 10 respectively while diameter of cylinder representing pores were chosen to be  $D = 1 \mu\text{m}$ .

In the two-phase FCC porosity cell, there is one spherical porosity at each corner and one spherical porosity in each face of the cube cell as shown in Fig. 1. Model consisting

multi-pore in unit cell (MPUC) differs from previous mentioned by the fact that number of pores with fixed aspect ratio of  $L/D$  and pores orientation is randomly chosen. This fact contributes to as close as possible real microstructure representation.



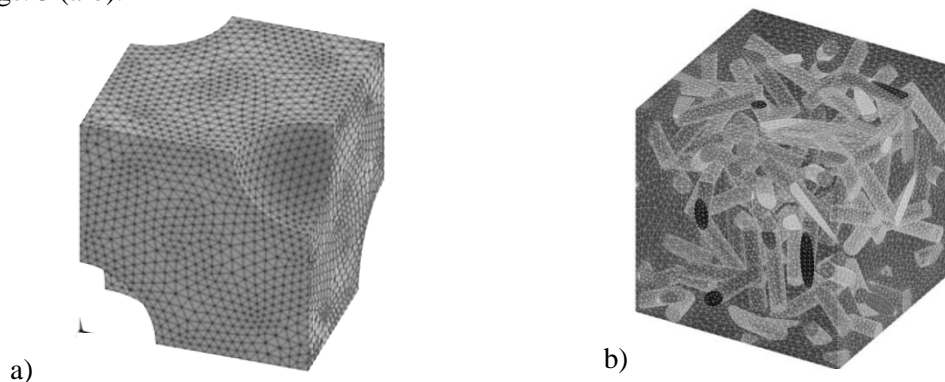
**Fig. 1.** Idealization of the random pore distribution, shape and size by arranging the pores on a FCC packing array.



**Fig. 2.** MPUC model with 10 % of porosity volume fraction ( $V_p$ ): (a)  $L/D=1$ , (b)  $L/D=5$ , (c)  $L/D=10$  and (d) dimensions of cylinder ( $D$ -diameter,  $L$ -length).

The assumptions for both models are: (I) the elastic properties of material are linear, (II) the material is isotropic, (III) all spherical and cylinder like pores are of the same size, (IV) the material will not fail at the prescribed loads and (V) pores do not intersect each other.

Due to the symmetry of the unit cell and the applied loads, as well as adopted isotropic material properties, the models were reduced to one eighth of the unit cell, as shown in Figs. 3 (a-b).



**Fig. 3.** FE grid of unit cell with 13.4 % of porosity volume fraction ( $V_p$ ): (a) FCC model and (b) MPUC model.

The models are considered by introducing boundary conditions, which constrains the unit cell to remain in its original shape (cube). After loading, the sides remain parallel and orthogonal, but changes in length. The unit cell is loaded in compression along vertical – y direction with adequate displacement steps. The local coordinate system aligns with the global one. Dimensions of reduced unit cells presented at Fig. 2 are:  $30 \times 30 \times 30 \mu\text{m}$ . All 3D FE models were produced using ANSYS 16.4, a general purpose finite element software package for structural analysis. The elements used are 10-node tetrahedral structural solid elements (an option of 20-node solid brick elements). A representative FE grid for evaluation of compressive stiffness with porosity volume fraction  $V_p = 0.134$ , shown in Fig. 3 (a), contains 67453 elements and 95764 nodes. Each node has three degrees of freedom corresponding to the three degrees of translation. The material data used for FE analyses, adopted based on literature data [14], with following values:  $E = 16,04 \text{GPa}$ ,  $\nu = 0.124$ , where  $E$  is Young's modulus and  $\nu$  is Poisson's ratio.

It should be noticed that numerical simulations for MPUC models with aspect ratio  $L/D=10$  were restricted to an upper level of  $V_p=0.17$  since intersecting of pores dramatically increases which directly influence major condition that intersecting of cylinders- pores was not allowed. For other aspect ratios: 1, 2 and 5, numerical simulations for MPUC models were restricted to an upper level of  $V_p=0.2$ .

### 3. Results and Discussion

Using load in form of displacement  $\Delta=0,3 \mu\text{m}$  in vertical direction of the nodes positioned at upper surface of the cube ( $y = 30 \mu\text{m}$ ) Figs. 2 (a, b), with condition that side surfaces have to remain parallel to their original directions, values for  $E$ , and  $\nu$  were obtained using following equations:

$$E = \frac{FH}{\Delta A} \quad (1)$$

$$\nu = -\frac{\Delta^{\text{side}}}{\Delta} \quad (2)$$

where force  $F$  is obtained by summing reactions on the constrained surface, opposite to the loaded surface, area  $A$  is  $900 \mu\text{m}^2$ , cube dimension is  $H = 30 \mu\text{m}$  and displacement is  $\Delta= 0,3 \mu\text{m}$  in y direction. After deformation, lateral displacement is marked by  $\Delta^{\text{side}}$ . Poisson's ratio  $\nu$  is calculated from equation (2). For isotropic body, values for  $G$  and  $K$  can be calculated from following relations:

$$G = \frac{E}{2(1+\nu)} \quad (3)$$

$$K = \frac{E}{3(1-2\nu)} \quad (4)$$

For different aspect ratios, values of compressive Young's modulus of elasticity ( $E$ ), shear modulus ( $G$ ) and bulk modulus ( $K$ ) were calculated by equations (1), (3) and (4).

Numerical solutions for different volume fractions of pores obtained by MPUC model for different aspect ratios are presented in Figs. 4, 5 and 6.

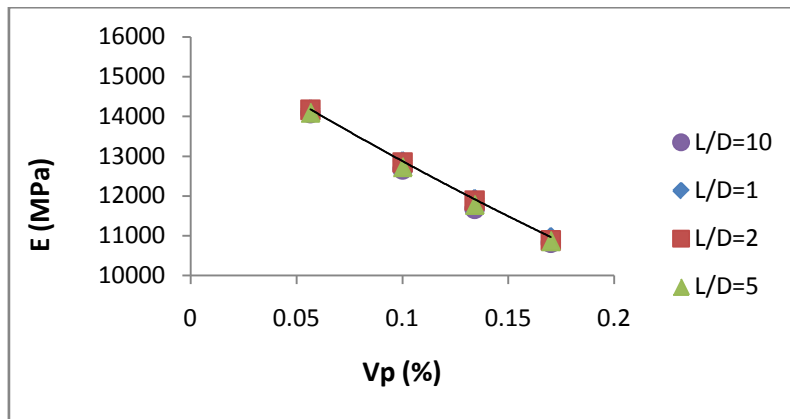


Fig. 4. Comparison of obtained values of E for different aspect ratios.

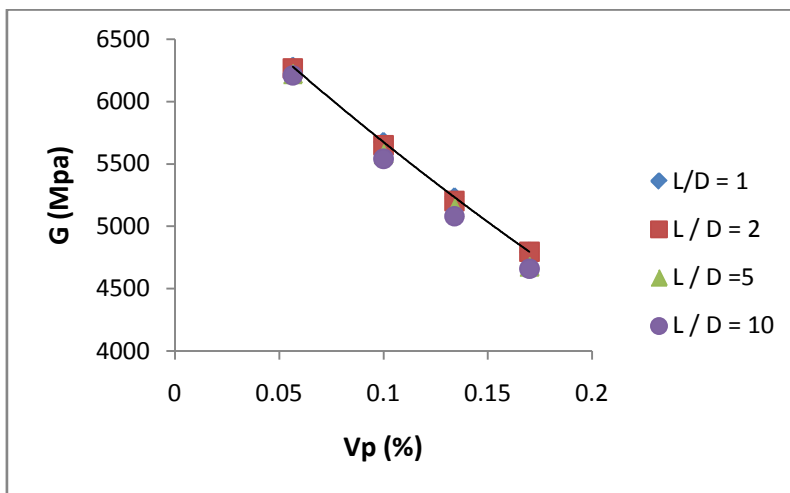


Fig. 5. Comparison of obtained values of G for different aspect ratios.

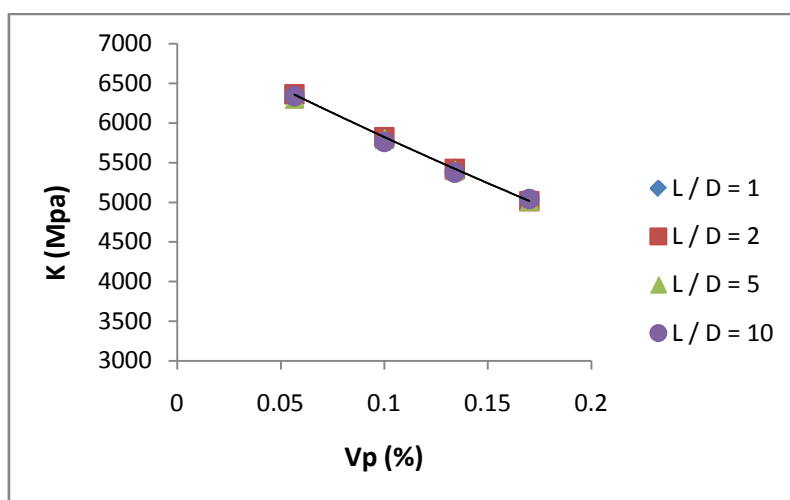


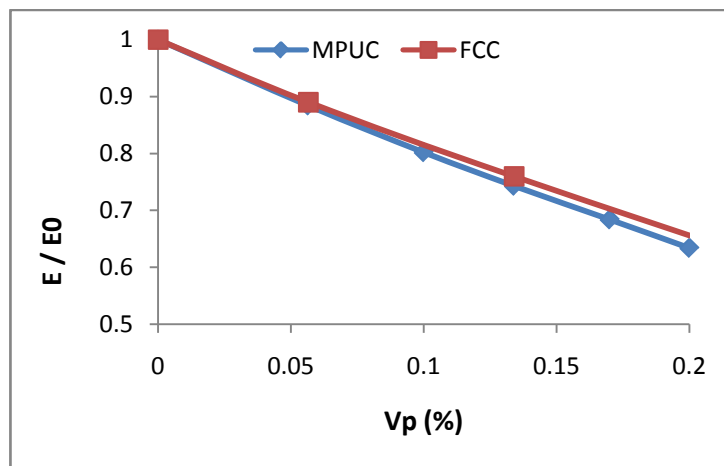
Fig. 6. Comparison of obtained values of K for different aspect ratios.

Summary of obtained results for E, G and K for different aspect ratios (1, 2, 5 and 10) are presented at Table 1.

Numerical solutions for different volume fractions of pores of compressive Young's modulus of elasticity –E obtained by FCC and MPUC models were compared at Fig 7. Values of normalized values for modulus of elasticity presented for MPUC are averaged values obtained for all aspect ratios considered. As obvious from presented results, MPUC model slightly underestimates values for modulus of elasticity when comparing to values obtained by FCC model.

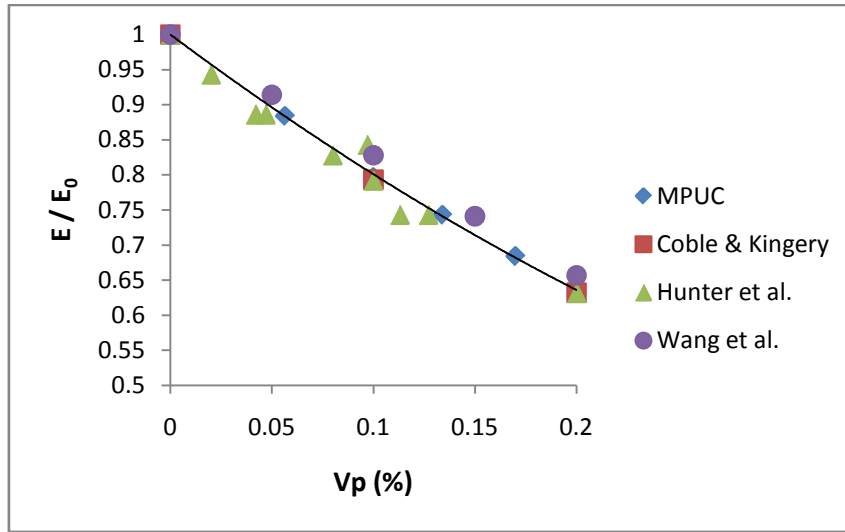
**Tab. I** Summary of obtained results for E, G and K for different aspect ratios.

L/D = 1				
Porosity volume fraction $V_p$ (%)	5.65	10	13.4	17
Modulus of elasticity E (MPa)	14180	12873	11924	10968
Shear modulus G (MPa)	6279	5676	5233	4795
Bulk modulus K (MPa)	6356	5818	5423	5016
L/D = 2				
Porosity volume fraction $V_p$ (%)	5.65	10	13.4	17
Modulus of elasticity E (MPa)	14166	12844	11884	10886
Shear modulus G (MPa)	6265	5651	5203	4747
Bulk modulus K (MPa)	6361	5821	5420	5015
L/D = 5				
Porosity volume fraction $V_p$ (%)	5.65	10	13.4	17
Modulus of elasticity E (MPa)	14100	12733	11784	10869
Shear modulus G (MPa)	6221	5581	5147	4679
Bulk modulus K (MPa)	6307	5799	5406	5020
L/D = 10				
Porosity volume fraction $V_p$ (%)	5.65	10	13.4	17
Modulus of elasticity E (MPa)	14086	12671	11676	10822
Shear modulus G (MPa)	6209	5541	5081	4661
Bulk modulus K (MPa)	6338	5761	5375	5043

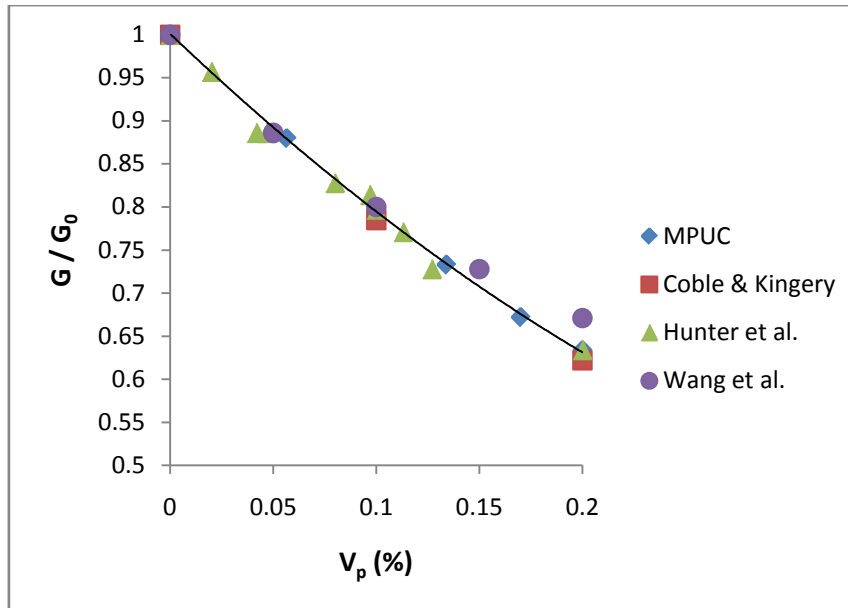


**Fig. 7.** Numerical solutions for different volume fractions of pores of normalized compressive Young's modulus of elasticity –E obtained by FCC and MPUC models.

Additionally, obtained results are compared to the experimental values available at literature [10, 15-17], as presented at Figs. 8 and 9.



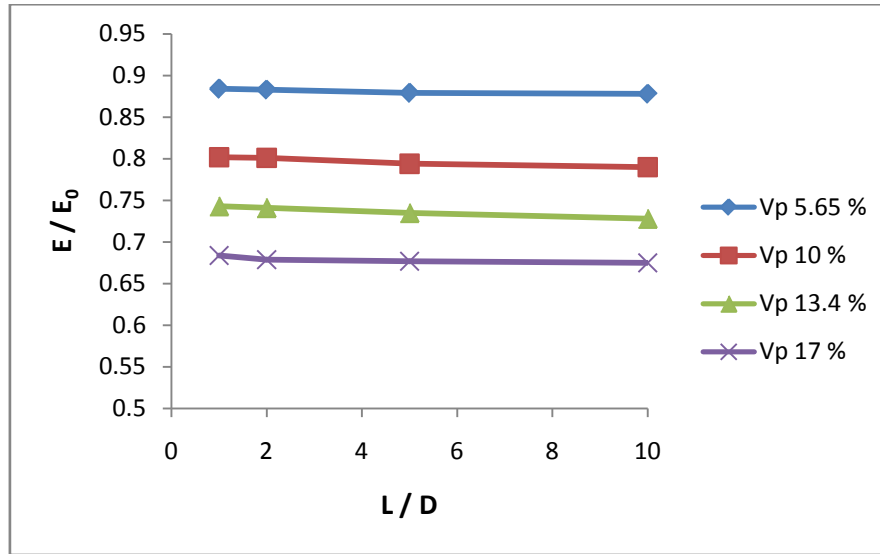
**Fig. 8.** Comparison of obtained results for E with experimental data from literature: Coble and Kingery [15], Hunter et al. [17] and Wang et al. [10].



**Fig. 9.** Comparison of obtained results for G with experimental data from literature: Coble and Kingery [15], Hunter et al. [17] and Wang et al. [10].

As it is evident, with the increase in porosity content compressive modulus significantly decreases, for example, porosity of 10 % leads to a modulus of elasticity decrease of approximately 20 %. The other two modulus decrease is similar.

Fig. 10 presents influence of pores shape (L/D) to Young's modulus of elasticity - E for fixed different porosity volume fractions - V<sub>p</sub>.



**Fig. 10.** Influence of pores shape ( $L/D$ ) to Young's modulus of elasticity -  $E$  for different fixed porosity volume fractions -  $V_p$ .

As it is evident from Fig. 10, shape of porosity has a slight impact on modulus of elasticity –  $E$  by slightly lowering its value with increasing aspect ratio ( $L/D$ ) of pore. Same trend is observed for the other two elastic constants  $G$  and  $K$ . It can be concluded that this influence is negligible when comparing to influence of volume fraction which is dominant.

#### 4. Conclusion

A 3D MPUC FE model of low level porosity is developed and compared with 3D FCC unit cell model as well as available experimental results. The low-level porosity has noticeable influence on the sintered material elastic properties: modulus of elasticity -  $E$ , shear modulus -  $G$  and bulk modulus -  $K$ . Shape of porosity has a low level impact on elastic properties. For fixed volume fraction, changing shape of pores by increasing aspect ratio ( $L/D$ ) slightly decreases values for  $E$ ,  $G$  and  $K$  and therefore has no significant influence on elastic characteristics. Volume fraction of porosity has a significant impact on material elastic properties. Less porosity in the material microstructure generally leads to noticeable higher values of  $E$ ,  $G$  and  $K$ . It is shown that values of effective elastic and shear moduli predicted by MPUC model are in excellent agreement with several sets of previously published experimental data. Comparisons with other existing numerical model - FCC have also shown very good agreement.

Finally, presented MPUC model are capable to simulate microstructure irregularity of pores shape and size regarding the influence of porosity volume fraction to elastic properties of porous material.

#### Acknowledgments

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**Садржај:** Утицај порозитета на еластичне карактеристике синтерованих материјала је разматран применом новог *multi-pore unit cell* - MPUC нумеричког модела. Извршено је поређење резултата за модул еластичности -  $E$ , модул смицања -  $G$  и запремински модул -  $K$ , добијених применом MPUC нумеричког модела као и применом претходно развијеног двофазног FCC нумеричког модела са резултатима добијеним експерименталним путем на основу података добијених из раније публикованих радова. Предложени MPUC модел даје резултате за  $E$ ,  $G$  и  $K$  за различите запреминске уделе порозитета који се изузетно добро поклапају са експерименталним подацима. Потврђено је да материјална порозност са својом величином (запреминским уделом) значајно утиче на еластичне карактеристике синтерованог материјала. Мања порозност у микроструктури материјала доприноси значајном повећању вредности за  $E$ ,  $G$  и  $K$ . Са друге стране, сам облик порозитета нема значајнијег утицаја на еластичне карактеристике за одређени запремински удео порозитета.

**Кључне речи:** Модул еластичности, Модул смицања, Запремински модул, Порозитет, Синтеровани материјали.

