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Modeling the effect of porosity and pore morphology on the mechanical properties of titanium structures for osteosynthesis

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Abstract. In this study, numerical modeling of porous titanium structures intended for use in osteosynthesis systems was performed using the finite element method. The main objective of the work was to evaluate the mechanical behavior of porous structures with different pore geometrical parameters and levels of porosity. For this purpose, representative volume elements (RVE) were constructed, representing fragments of the porous structure. These elements were analyzed under uniaxial loading in order to determine the distribution of stresses and strains within the material. During the simulations, several structural variants with different porosity levels and pore sizes were examined. The obtained results demonstrated that porosity is a key parameter that significantly influences the mechanical behavior of the material. With increasing porosity, a rise in stress concentration in the struts between pores was observed, along with increased heterogeneity of stress and strain fields. This effect is associated with the reduction of the effective load-bearing cross-sectional area of the material and the redistribution of loads within the structure. Analysis of the stress–strain curves for models with pore sizes of 200, 400, and 600 μm showed that, at a fixed level of porosity, variation in pore size has a relatively minor effect on the effective elastic modulus of the material. At the same time, it was established that the geometrical shape of the pores has a more significant impact on the mechanical properties of the structure, including stiffness and stress distribution. The obtained results confirm that optimization of pore geometry is an important factor in the design of porous titanium implants aimed at improving their biomechanical compatibility with bone tissue.

Keywords: *porous titanium structures, osteosynthesis, porosity, finite element method, mechanical properties.*

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1. Introduction

In modern orthopedics, metallic and biodegradable materials are primarily used for the internal fixation of limb fractures. However, the elastic modulus of metallic materials (such as stainless steel, titanium, and its alloys) differs significantly from that of human bone tissue [1-3]. The elastic modulus of cast titanium is approximately 100 GPa, while that of the widely used titanium alloy Ti6Al4V is about 110 GPa [4-6].

In contrast, the elastic modulus of human bone ranges from 15 to 30 GPa and depends on factors such as sex, age, and overall health condition [7-9]. The difference in elastic modulus between human bone and titanium implants leads to the so-called stress shielding effect, which may necessitate revision surgery [10, 11]. The mismatch between the high elastic modulus of implants and the biomechanical properties of bone negatively affects callus formation and fracture healing, potentially requiring additional surgical intervention [4, 5].

Therefore, the development of internal fixation systems that do not require secondary surgery for removal has remained an important research topic in the orthopedic community for many years [7, 8]. To reduce the elastic modulus of metallic materials, researchers have investigated porous materials for use in medical metallic implants [9].

The porous architecture of implants plays a key role in determining their mechanical and biological properties. It has been established that increasing porosity promotes improved osseointegration and bone tissue ingrowth; however, it simultaneously leads to a reduction in the strength and stiffness of the material. Therefore, optimization of the parameters of porous structures, including the level of porosity, pore size, and pore morphology, represents an important task in the design of implants for osteosynthesis [12].

Porous materials used for implants in the treatment of bone injuries and defects typically require a porosity ranging from approximately 30% to 85%. In such materials, the pores should preferably be interconnected and uniformly distributed; alternatively, depending on specific requirements, a portion of the pores may be interconnected while still maintaining a uniform distribution. This structural configuration facilitates effective integration of the material with human bone tissue [9, 11].

Currently, a number of technologies have been developed that enable the fabrication of porous titanium structures with different morphologies, pore sizes, and levels of mechanical strengths. Figure 1 illustrates porous titanium structures used in orthopedic applications.

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Figure 1. Orthopedic devices made of porous titanium

Porous titanium can be produced using additive manufacturing technologies such as Selective Laser Melting (SLM) and Electron Beam Melting (EBM), powder metallurgy methods, space-holder techniques, Binder Jetting, as well as technologies for producing metallic foams and combined gradient structures [13-15]. In addition, porous structures can be fabricated using Spark Plasma Sintering and open-cell architectures. However, the aforementioned porous materials often exhibit characteristics such as small pore sizes, non-uniform pore distribution, poor permeability, or the presence of numerous micropores within the pore wall structure, which may hinder their application as biomaterials [16-18].

When developing modern implant materials, particular attention is given to their elastic modulus, compressive strength, and biocompatibility [19-20].

In recent years, the development of porous metallic structures has become one of the most promising directions in biomedical engineering and orthopedics. In this context, numerical modeling of porous structures using the Finite Element Method has gained particular importance. Nevertheless, many porous materials produced by the aforementioned methods still possess limitations, including small pore sizes, non-uniform pore distribution, low permeability, or the presence of numerous micropores in the pore wall structure [21-23].

Such structural features can significantly limit their application as biomaterials. Moreover, they may negatively affect both the mechanical properties of the material and the processes of osseointegration, since insufficient pore interconnectivity and improper pore geometry hinder bone tissue ingrowth and reduce the transport of nutrients and cells within the implant [24].

In this context, optimization of the porous architecture becomes particularly important, including the control of pore size, shape, distribution, and the overall level of porosity. Experimental investigation of all possible pore geometry variations is a complex, time-consuming, and costly process. Therefore, in recent years numerical modeling of porous structures using computer simulation and the Finite Element Method has become increasingly widespread (Design, Modeling, Additive Manufacturing, and Polishing of Stiffness-Modulated Porous Nitinol Bone Fixation Plates Followed by Thermomechanical and Composition Analysis).

Modeling makes it possible to analyze in detail the influence of porous architecture parameters on the stress–strain state of the material, evaluate the distribution of stresses and strains within the structure, and predict the effective mechanical properties of porous constructions. The application of such approaches significantly accelerates the design process of biomedical implants and allows the determination of optimal parameters of porous structures that provide the required combination of strength, stiffness, and biological compatibility (Novel Clinical Applications of 3D-Printed Highly Porous Titanium for Off-the-Shelf Cementless Joint Replacement Prostheses).

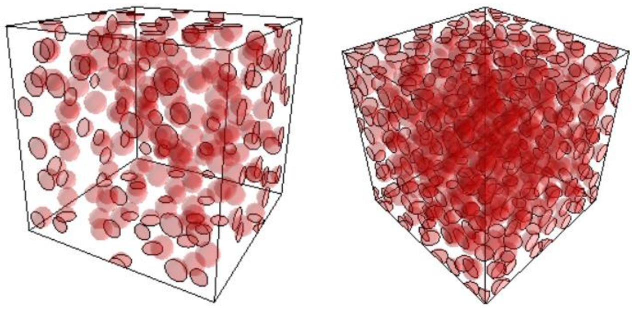
Based on the relevance of the studies mentioned above, this work conducts computational experiments using the DIGIMAT software in order to identify the relationships between porosity, pore size, and pore shape and their influence on the elastic modulus of titanium.

2. Materials and methods

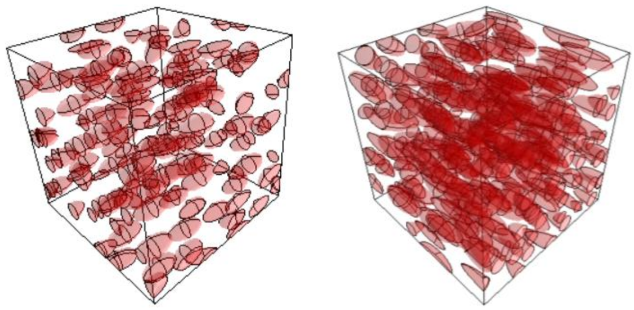
The numerical investigation of the effects of porosity, pore size, and pore morphology on the mechanical properties of titanium material was performed using the DIGIMAT MF/FE software, designed for multiscale modeling of heterogeneous media. In the study, a micromechanical model of a Representative Volume Element (RVE) was employed, enabling consideration of the influence of the material's internal structure on its effective mechanical properties.

The matrix material was the titanium alloy Ti-6Al-4V, whose mechanical properties were defined using a linear-elastic isotropic model. The parameters used in the simulations were: elastic modulus $E = 110$ GPa, Poisson's ratio $\nu = 0.33$, and density $\rho = 4430$ kg/m^3. Pores were modeled as inclusions with zero stiffness and zero density, corresponding to the idealized case of a completely void volume.

Porosity was varied within a specified range to assess its effect on the material's effective elastic properties. Pore size was defined using a characteristic linear parameter of the inclusions at a fixed volume fraction, while pore shape was modeled as spherical, ellipsoidal, and cellular (architected) structures. Figure 2 illustrates the pore parameters and their orientations.



(a) (b)



(c) (d)

Figure 2. Representative volume element of a titanium matrix filled with pores: (a) spherical pores with 30% porosity; (b) spherical pores with 50% porosity; (c) ellipsoidal pores with 30% porosity; (d) ellipsoidal pores with 50% porosity

During modeling, three main structural parameters were varied: the volume fraction of pores (porosity), pore size, and pore shape. Table 1 presents the parameter variations used in the computational experiments.

Table 1. Parameters of the computational experiment

№	Porosity, %	Pore size	Pore shape
1	30	200/300/400	Sphere / Ellipsoid
2	40	200/300/400	Sphere / Ellipsoid
3	50	200/300/400	Sphere / Ellipsoid
4	60	200/300/400	Sphere / Ellipsoid

The calculations were performed using the finite element method in combination with a homogenization procedure [25, 26]. Boundary conditions were applied as uniform deformation of the representative volume element, ensuring the accurate determination of averaged stresses and strains. The simulations yielded the effective elastic modulus, Poisson's ratio, and stress distribution within the porous structure, and the influence of pore morphology on the material's mechanical behavior was analyzed. The obtained results were further used to assess the effect of pore morphology on the mechanical performance of porous titanium and to compare them with theoretical models such as the Gibson-Ashby model.

3. Results and discussion

First, the numerical experiment was conducted using the DIGIMAT MF module, modeling structures with different pore sizes while maintaining a constant solid-phase volume fraction. The calculations were performed under uniaxial tensile loading with a prescribed deformation, enabling assessment of the effect of pore morphology on the stress-strain response and the effective elastic modulus of the material. The results are presented in Figure 3.

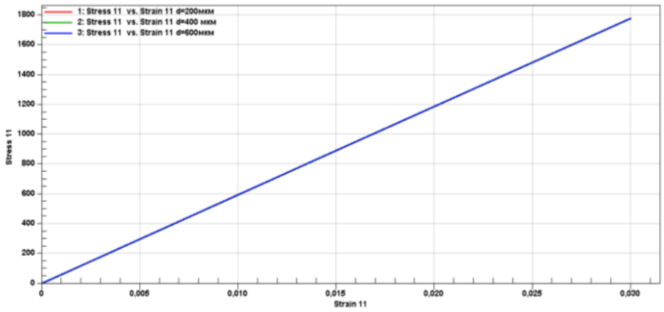
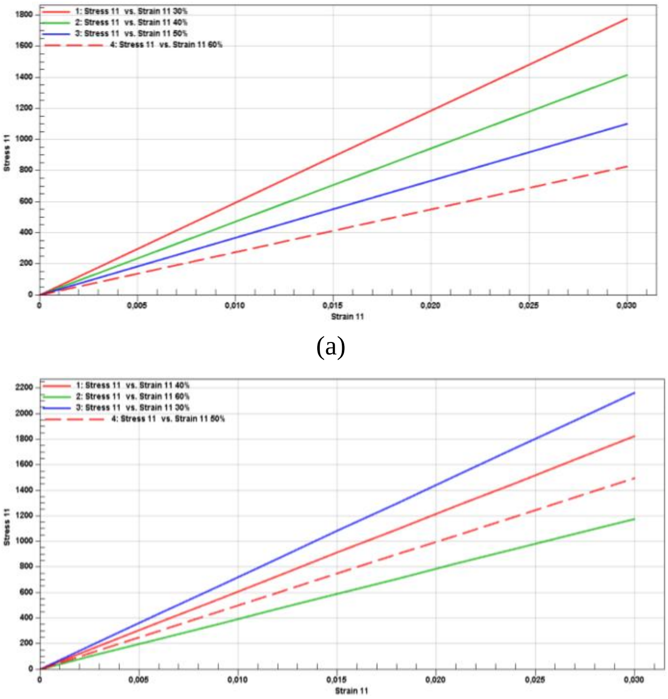


Figure 3. Stress-strain diagram for pore sizes of 200 µm, 400 µm, and 600 µm

All stress-strain curves exhibit nearly identical slopes, indicating that the elastic modulus is similar regardless of pore diameter. Next, calculations were performed in the DIGIMAT MF module for different pore shapes, ellipsoidal and spherical, at varying porosity levels as specified in Table 2. The results are presented in Figure 4

Table 2. Stress values (u = 0.01) and elastic modulus for different porosity levels and pore shapes

Porosity, %	Ellipsoidal aspect ratio 6		Spherical aspect ratio 1	
	σ, MPa	*E*, GPa	σ, MPa	*E*, GPa
30	700	58.5	600	59
40	600	47	450	47.1
50	500	36.8	380	36.6
60	400	27.94	280	27.5



(b)

Figure 4. Tensile stress-strain diagram (u = 0.01) with pore diameter 200 µm; (a) spherical pores, (b) ellipsoidal pores

Apparent differences in the slopes of the stress-strain curves are observed for the two pore shapes.

Despite differences in pore geometry, the effective elastic modulus of porous titanium with ellipsoidal and spherical pores at the same porosity is similar. This can be explained by the fact that the elastic modulus is an integral material property, primarily determined by the volume fraction of the solid phase rather than the local pore shape. According to the Gibson-Ashby model, the effective elastic modulus of porous and cellular materials is described by the following expression [27]:

$$E = E_S \left(1-\varphi\right)^n , \quad (1)$$

where E_s is the elastic modulus of the dense material; φ is the porosity; n is the exponent determined by the type of cellular structure and the deformation mechanism.

At a fixed porosity, the influence of pore shape on the global stiffness of the material is secondary. However, pore geometry has a significant effect on the local stress distribution: ellipsoidal pores exhibit higher stress concentrations due to their smaller radius of curvature and pronounced anisotropy, leading to higher equivalent stresses than spherical pores. Thus, for the same effective elastic modulus, differences in the stress state are primarily attributed to stress concentration effects rather than changes in the bulk elastic properties of the material [28, 29].

Third, finite element modeling was performed using the DIGIMAT FE module. Figure 5 shows the distribution of equivalent stresses obtained from the finite element analysis of a porous titanium structure in DIGIMAT FE. The calculations were carried out for a representative volume element with specified porosity and pore size under uniaxial loading. The visualization enables analysis of stress distribution within the material volume and identification of stress concentration zones resulting from the porous structure's geometry.

(a)

(b)

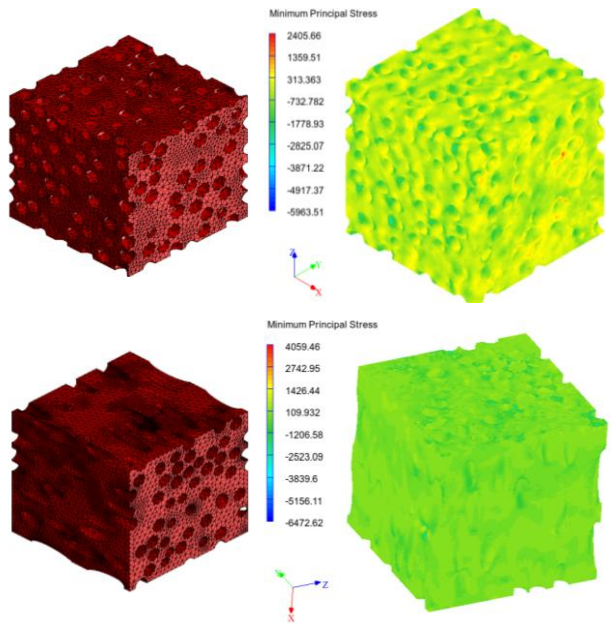


Figure 5. Distribution of equivalent stresses in a porous titanium structure under uniaxial loading (porosity 30%, pore size 200 µm): (a) with a spherical pore, (b) with an ellipsoidal pore

The numerical modeling of stress distribution in the representative volume of porous titanium revealed that the local components of the stress tensor reach 2405 MPa for spherical pores and 4059 MPa for ellipsoidal pores, due to stress concentration in the ligaments between pores. At the same time, the volume-averaged stresses remain significantly lower than the local maxima, confirming the validity of the homogenization approach.

Physically, stresses in the material concentrate in regions with abrupt changes in geometry or small radii of curvature. For spherical pores, the radius of curvature is uniform in all directions, resulting in a more even stress distribution. In contrast, ellipsoidal pores have sharp regions (small radius of curvature at the ends of the ellipse), leading to substantial stress concentrations.

4. Conclusions

In finite element modeling, titanium models with varying porosity and pore diameter were used. According to our calculations, the most significant variable affecting stress concentration and the heterogeneity of the stress-strain field is matrix porosity. Analysis of the stress-strain response for different pore sizes (200, 400, and 600 µm) showed that, at a fixed porosity, changes in pore size have a negligible effect on the effective elastic modulus of the material. Further analysis of the modeling results indicated that, while pore size has little influence on mechanical properties at a fixed porosity, pore shape, as reflected in the aspect ratio, is the key factor. It was found that as the deviation from spherical pore shape increases (i.e., higher aspect ratio), the effective mechanical properties, particularly the elastic modulus, decrease.

To achieve optimal properties for titanium implants, a new design of porous titanium with gradient porosity is proposed. Future work will focus on the development and testing of advanced materials intended for biomedical applications.

Author contributions

Conceptualization: MI, EI; Data curation: GS, AD; Formal analysis: MI, EI, AD; Funding acquisition: MI, AT; Investigation: GS, AT; Methodology: AD, EI; Project administration: MI, AT; Resources: GS, MI; Software: EI, AD; Supervision: MI, GS; Validation: EI, AT; Visualization: EI, MI; Writing – original draft: MI, AT; Writing – review & editing: MI, AT. All authors have read and agreed to the published version of the manuscript.

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Conflicts of interests

The authors declare no conflict of interest.

Data availability statement

The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

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Остеосинтезге арналған титан құрылымдарының механикалық қасиеттеріне кеуектілік пен кеуектер морфологиясының әсерін модельдеу

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Аңдатпа. Осы зерттеуде остеосинтез жүйелерінде қолдануға арналған кеуекті титан конструкцияларын сандық модельдеу Finite Element Method (соңғы элементтер әдісі) негізінде жүргізілді. Жұмыстың негізгі мақсаты – кеуектердің әртүрлі геометриялық параметрлері мен кеуектілік деңгейлері жағдайында кеуекті құрылымдардың механикалық мінез-құлқын бағалау болды. Осы мақсатта кеуекті құрылымның фрагменттерін сипаттайтын өкілдік көлемдік элементтер – Representative Volume Element (RVE) қалыптастырылып, материал ішіндегі кернеулер мен деформациялардың таралуын анықтау үшін олар біросьтік жүктеме жағдайында талданды. Модельдеу барысында кеуектіліктің әртүрлі деңгейлері мен кеуек өлшемдері бар құрылымдардың бірнеше нұсқасы қарастырылды. Алынған нәтижелер кеуектілік материалдың механикалық мінез-құлқына шешуші әсер ететін негізгі параметр екендігін көрсетті. Кеуектілік артқан сайын кеуектер арасындағы байланыс аймақтарында кернеулердің шоғырлануы өсетіні, сондай-ақ кернеу мен деформация өрістерінің біркелкі еместігі күшейетіні байқалды. Бұл құбылыс материалдың тиімді жүк көтеретін қимасының азаюымен және құрылым ішіндегі жүктемелердің қайта бөлінуімен түсіндіріледі. Кеуек өлшемдері 200, 400 және 600 мкм болатын модельдер үшін кернеу–деформация тәуелділігі қисықтарын талдау нәтижесінде кеуектілік деңгейі тұрақты болған жағдайда кеуек өлшемінің өзгеруі материалдың тиімді серпімділік модуліне салыстырмалы түрде аз әсер ететіні анықталды. Сонымен қатар кеуектердің геометриялық пішіні құрылымның механикалық қасиеттеріне, соның ішінде қаттылығына және кернеулердің таралуына едәуір ықпал ететіні анықталды. Алынған нәтижелер кеуекті титан имплантаттарын жобалау кезінде олардың сүйек тінімен биомеханикалық үйлесімділігін арттыру мақсатында кеуек пішінін оңтайландыру маңызды фактор болып табылатынын растайды.

Негізгі сөздер: *кеуекті титан құрылымдары, остеосинтез, кеуектілік, соңғы элементтер әдісі, механикалық қасиеттер.*

Моделирование влияние пористости и морфологии пор на механические свойства титановых структур для остеосинтеза

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Аннотация. В данном исследовании было проведено численное моделирование пористых титановых конструкций, предназначенных для применения в системах остеосинтеза, с использованием метода конечных элементов. Основной целью работы являлась оценка механического поведения пористых структур при различных геометрических параметрах пор и уровнях пористости. Для этого были сформированы характерные объемные элементы (Representative Volume Element, RVE), представляющие собой фрагменты пористой структуры, которые анализировались при одноосной нагрузке с целью определения распределения напряжений и деформаций в материале. В ходе моделирования были рассмотрены несколько вариантов структуры с различными уровнями пористости и размерами пор. Полученные результаты показали, что пористость является ключевым параметром, оказывающим определяющее влияние на механическое поведение материала. При увеличении пористости наблюдается рост концентрации напряжений в перемычках между порами, а также повышается неоднородность полей напряжений и деформаций. Это связано с уменьшением эффективной площади несущего сечения материала и перераспределением нагрузок внутри структуры. Анализ кривых зависимости напряжения от деформации для моделей с размерами пор 200, 400 и 600 мкм показал, что при фиксированном уровне пористости изменение размера пор оказывает сравнительно незначительное влияние на эффективный модуль упругости материала. В то же время установлено, что геометрическая форма пор оказывает более существенное влияние на механические свойства структуры, включая жесткость и распределение напряжений. Полученные результаты подтверждают, что оптимизация формы пор является важным фактором при проектировании пористых титановых имплантатов для улучшения их биомеханической совместимости с костной тканью.

Ключевые слова: *пористые титановые конструкции, остеосинтез, пористость, метод конечных элементов, механические свойства.*

Publisher's note