Vestnik of Don State Technical University. 2019. Vol. 19, no. 3, pp. 281–289. ISSN 1992-5980 eISSN 1992-6006
Вестник Донского государственного технического университета. 2019. Т. 19, № 3. С. 281–289. ISSN 1992-5980 eISSN 1992-6006

INFORMATION TECHNOLOGY, COMPUTER SCIENCE, AND MANAGEMENT
ИНФОРМАТИКА, ВЫЧИСЛИТЕЛЬНАЯ ТЕХНИКА И УПРАВЛЕНИЕ

UDC 004.94: 621.01 https://doi.org/10.23947/1992-5980-2019-19-3-281-289

The problem of mathematical finite element modeling of inhomogeneous deformable solids using scanning[*]

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Проблема математического конечноэлементного моделирования неоднородных деформируемых твердых тел с применением сканирования[***]

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Introduction. In the mathematical finite element modeling, an average value of the mechanical characteristics of the deformable solid material is used. In aircraft, machine building, construction engineering, medicine and other fields, polymer composite materials and materials of natural origin are increasingly used. In the latter case, the actual change in the mechanical characteristics differs significantly from the averaged change; therefore, when using the averaged parameters to build and analyze finite element models, the results can be significantly distorted. This paper describes the creation of mathematical methods for studying changes in the mechanical characteristics of a material of inhomogeneous deformable solids. The results obtained in this way are used to construct finite element models and analyze their stress-strain state.
Materials and Methods. Naturally occurring materials and composites are considered as inhomogeneous deformable solids. To study the changes in the mechanical characteristics of the material, a method was developed based on the use of two components: the pixel characteristics of raster images scanned by a computer tomograph and the experimental data of field tests of standard samples.
Research Results. A complex of mathematical methods has been developed for modeling the interpretation of scanning raster images by a computer tomograph, which allows for the study of any complicated structures of real deformable solids. The results are used in the construction of finite element models of such bodies considering the heterogeneity of the mechanical characteristics of the material. The analysis of the stress-strain state of finite element models of test samples has

Введение. При математическом конечноэлементном моделировании используется усредненное значение механических характеристик материала деформируемых твердых тел. В авиа-, машиностроении, строительстве, медицине и других областях все шире применяются полимерные композитные материалы и материалы природного происхождения. В последнем случае реальное изменение механических характеристик значительно отличается от усредненного, следовательно, при использовании усредненных параметров для построения и анализа конечноэлементных моделей результаты могут существенно искажаться.
В данной статье описано создание математических методов исследования изменения механических характеристик материала неоднородных деформируемых твердых тел. Полученные таким образом результаты применены для построения конечноэлементных моделей и анализа их напряженно-деформированного состояния.
Материалы и методы. В качестве неоднородных деформируемых твердых тел рассмотрены материалы природного происхождения и композиты. Для исследования изменения механических характеристик материала разработан способ, основанный на использовании двух составляющих: пиксельной характеристики растровых изображений сканирования компьютерным томографом и экспериментальных данных натурных испытаний стандартных образцов.
Результаты исследования. Создан комплекс математических методов моделирования интерпретации растровых изображений сканирования компьютерным томографом, позволяющий проводить исследование любых сложных структур реальных деформируемых твердых тел. Результаты используются при построении конечноэлементных моделей таких тел с учетом неоднородности механических характеристик материала.
Анализ напряженно-деформированного состояния конечноэлементных моделей тестовых образцов доказал точность и сходимость численного решения метода конечных

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proved the accuracy and convergence of the numerical solution of the finite element method in modeling the property of heterogeneity of the mechanical characteristics of the material.
Discussion and Conclusions. The developed approach can be applied to any physical principles of scanning (X-ray, ultrasound, laser, etc.) and for any types of materials if the data obtained as a result of scanning is developed in the form of a digital (raster) image.

элементов при моделировании свойства неоднородности механических характеристик материала.
*Обсуждение и заключения***.** Разработанный подход может быть применен для любых физических принципов сканирования (рентгеновский, ультразвуковой, лазерный и др.) и для любых типов материалов, если информация, полученная в результате сканирования, сформирована в виде цифрового (растрового) изображения.

Keywords: finite element method, deformable solid, inhomogeneity, mechanical properties of material.

Ключевые слова: метод конечных элементов, деформируемое твердое тело, неоднородность, механические характеристики материала.

For citation: Duong, V.L. The problem of mathematical finite element modeling of inhomogeneous deformable solids using scanning. Vestnik of DSTU, 2019, vol. 19, no. 3, pp. 281−289. https://doi.org/10.23947/1992-5980-2019-19-3-281-289

***Образец для цитирования*:** Зыонг, В. Л. Проблема математического конечноэлементного моделирования неоднородных деформируемых твердых тел с применением сканирования // Вестник Дон. гос. техн. ун-та. — 2019. — Т. 19, № 3. — С. 281−289. https://doi.org/10.23947/1992-5980-2019-19-3-281-289

Introduction. In the finite element (FE) modeling, mechanical characteristics of the material of deformable solids (DS) are specified as an averaged value used for the whole model. For example, mechanical characteristics of steel are determined through tensile and compression tests of standard regular samples. This approach is acceptable for the design and engineering practice. However, in modern aircraft, engineering, construction, medicine and other fields, polymer composites and materials of natural origin are increasingly used. A real change in the mechanical characteristics of such materials differs drastically from an average value; therefore, when using average parameters to build and analyze finite element models, the results can be significantly distorted.

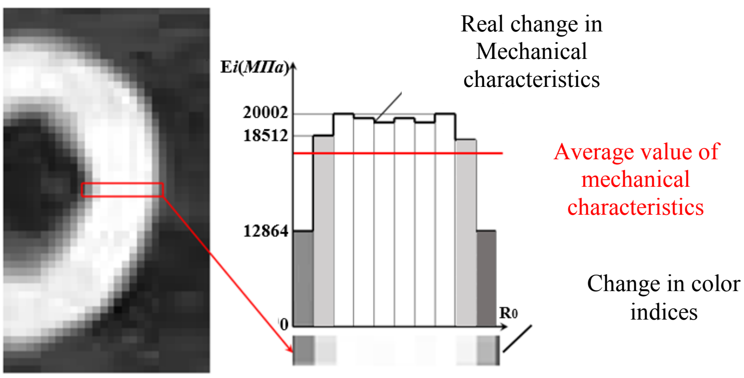
Research Results

1. The main mathematical dependence of modeling heterogeneity of real deformable solids. To solve the presented problem, a method for determining a real change in the mechanical characteristics of the material based on the use of:

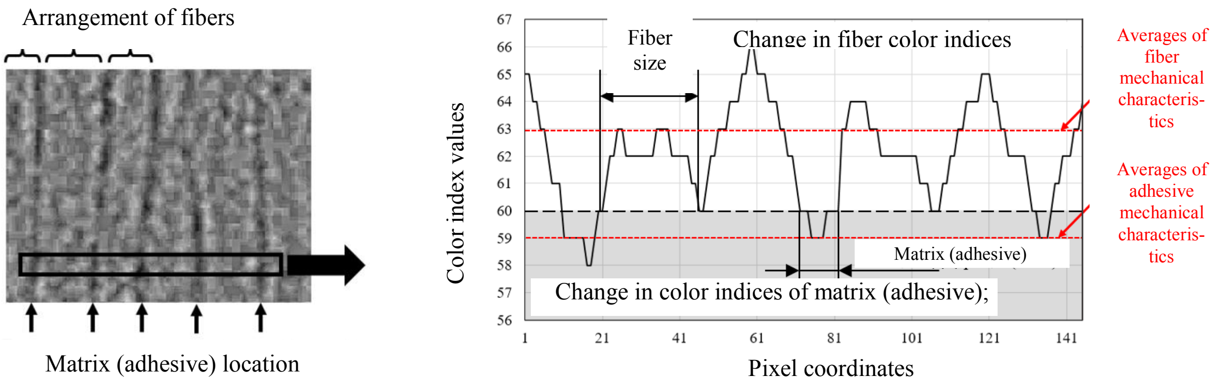
- DS scan results;
- data of field tests of standard samples [1].

This method makes it possible to recognize any complex heterogeneous material structure and apply this data to increase accuracy and realism in mathematical finite element modeling of real DS.

Fig. 1*a* shows an example of a raster image of scanning a material of natural origin (human bone). Its section demonstrates a change in mechanical characteristics depending on the values of the color indices (pixels) [2]. Fig. 1*b* shows the scan result of the composite material in the form of a raster image of the cross section of a regular sample (the scanning was performed by V.G. Tolstikov). Real changes in the mechanical characteristics of the fibers and matrix (adhesive) in the structure are indicated. In addition, the scanning has shown the possibility to assess quality of the composite materials (fiber arrangement, adhesive layer thickness, internal defects, etc.).



a)



b)

Fig. 1. Material of natural origin (*a*) and composite material (*b*) scan bitmap analysis

A general diagram of mathematical simulation and the algorithm of the proposed scanning technology are shown in Fig. 2 [2].

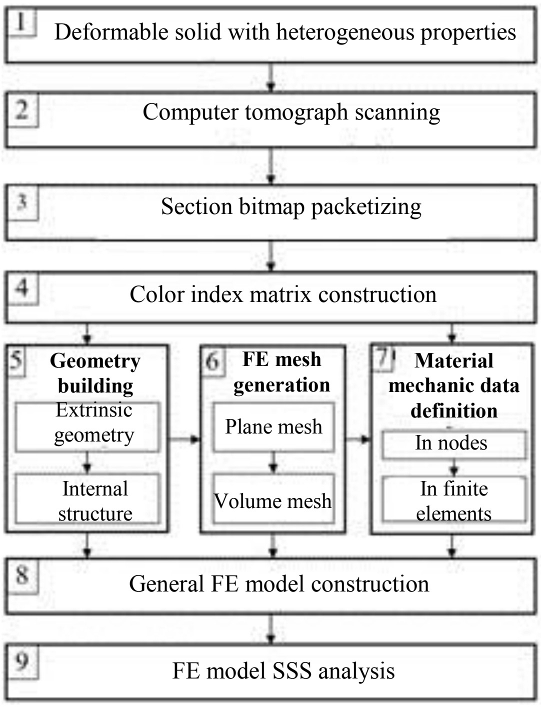


Fig. 2. Mathematical and finite element modeling of real deformable solids

The diagram reflects a full range of modules: from scanning DS to obtaining its FE model and analysis of the stress-strain state (SSS). If necessary, the cycle of operations is ensured within each block of the algorithm.

Scanning is performed using a computer tomograph (CT). When working with deformable objects, it provides image packetizing; each one is a raster image in a certain section [3, 4]. Standard raster image formats are jpeg, dicom, bmp, png, etc. Regardless of the format used, a raster image should be represented as a numerical matrix for further processing.

To determine the dependence of mechanical characteristics (for example, in the form of an elastic modulus) on the values of color indices, a special weight factor is applied [1], which establishes the relationship between the average value of the color indices n_{cp} and the experimental value $E_{ОП}$. The average value of the elastic modulus ($E_{ОП}$) obtained in the experiment on the tension (compression) of standard samples is used to interpret mechanical changes in the pixel characteristic.

Then the weight factor that determines the transition from the pixel color index to the elastic modulus is determined through an expression of the following form:

$$k_E = \frac{E_{ОП}}{n_{cp}} . \quad (1)$$

Here, n_{cp} is an average value of color indices of a scanning bitmap packet:

$$n_{cp} = \frac{\sum_{i=1}^{m}\sum_{j=1}^{n} I(i,j)}{mn}. \qquad (2)$$

However, for a large amount of CT SSS scan data with a high degree of the structure heterogeneity, it is required to use the mathematical expectation dependence when determining an average value of the color index. That is, n_{cp} is defined as an average value:

$$n_{cp} = E(n) = \sum_{i=1} n_i p_i(n_i), \qquad (3)$$

where n_i is the color index value on the interval I; $p_i(n_i)$ is the probability of occurrence of n_i (color index values) in the interval I.

Pixels, each of which has a corresponding color index, are assigned the values of the elastic modulus of the material E_i. For this, the weight factor k_E is used:

$$E_i = n_i k_E. \qquad (4)$$

Here, E_i is the elastic modulus value corresponding to the value of the color index number n_i; k_E is weight factor of the elastic modulus.

The dependence (4) for the FE model is implemented through solving the following tasks:

- determination of the dependence of mechanical characteristics on the values of color indices;

- determination of the mechanical characteristics of the material in the nodes and in the finite elements of the FE model.

A change in the elastic modulus is determined on the basis of a linear or non-linear dependence on the values of the color indices. For a material with a low degree of heterogeneity, the dependence can be constructed according to the linear law (4) using a single constant value of the weight factor of the elastic modulus.

However, such materials are rare in nature and engineering. Most often, several areas can be distinguished in the structure of a DS material, each of which has a different variation range of the elasticity modulus than the others.

It is proposed to apply a nonlinear law for such materials, which provides its own weight factor value in each region of the DS structure. In this case, the dependence of the change in the DS elastic modulus on the color indices is presented as a piecewise linear function (Fig. 3*a*).

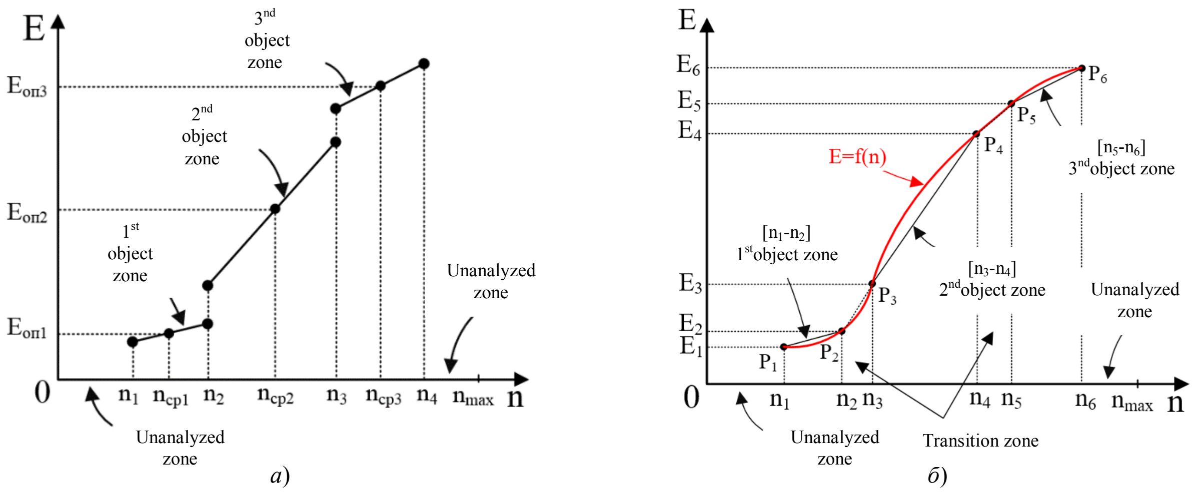


Fig. 3. Piecewise linear (*a*) and continuous (*b*) function of DS elasticity modulus variation from color index values

Using a piecewise linear function is difficult from the point of view of the computational algorithm efficiency, in particular, due to the following reasons:

- the larger the number of the DS structure regions, the greater the number of weight factors and the more complicated the calculation of the elastic modulus for nodes and finite elements;

- transition values of color indices between DS regions or objects involve not one value, but ranges of values of color indices in a bitmap (see Fig. 3*b*).

To solve this problem, a nonlinear dependence in the form of a spline, for example, a cubic one [5], can be constructed on the basis of a piecewise linear function. Such a nonlinear dependence of the DS elastic modulus on color indices is universal when combining several zones with different patterns of mechanical characteristics (see Fig. 3*b*).

Next, the interpretation of the scanning data is associated with the interpolation and transmission of color index values from pixels to the nodes of the FE mesh. In the most complex and general case, the FE nodes of the mesh lie between adjacent planes with a bitmap. They vary widely in shape and size. Besides, additional internal contours and other geometric features appear in them. In this case, a number of mathematical dependences are used for interpolation; they are determined with respect to a straight line inclined to the Z axis [6].

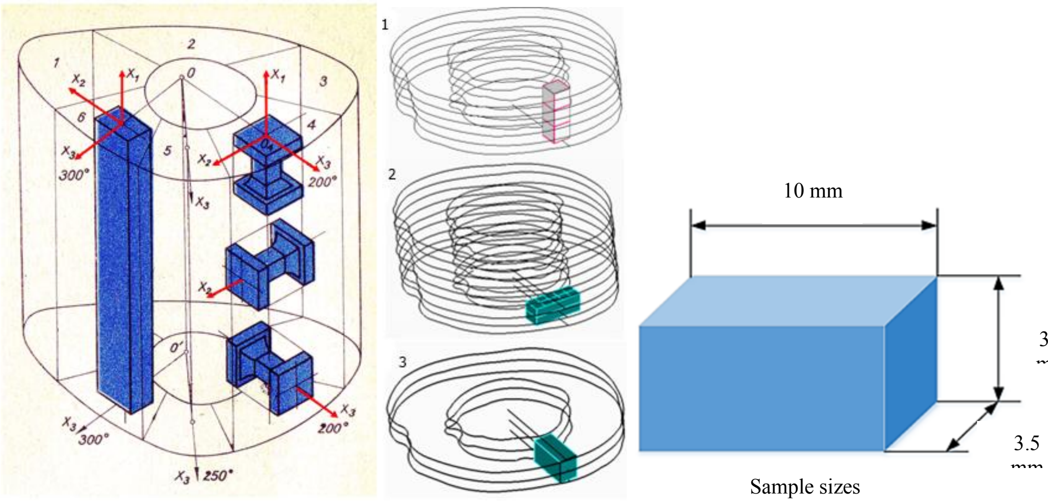
In [2], a more similar description of the mathematical dependence and the block diagram of the algorithm for determining the mechanical characteristics of the material in the nodes and finite elements of the DS FE model is presented (see Fig. 2, block 7).

To use the results of determining the heterogeneity of the material mechanical characteristics in the FE model, they are converted to a file with the **.pcl* extension. Two functions of the Patran Command Language: “material.create” and “elementprops_create” [7, 8] are used for this.

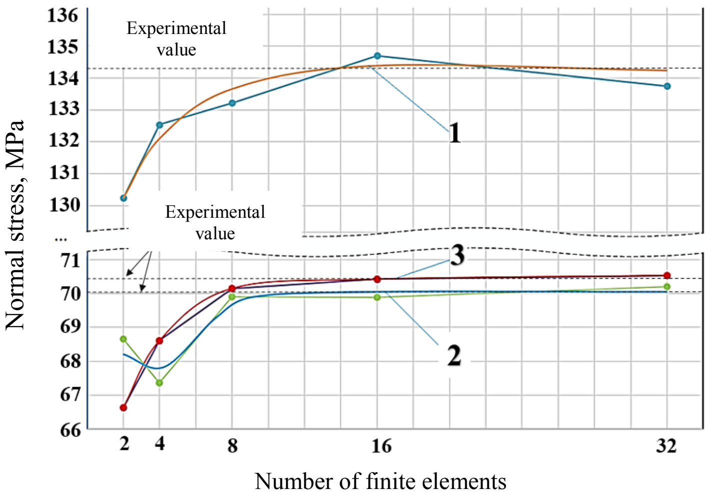
2. Investigation of the accuracy and convergence of the analysis results of the FE models considering simulation of heterogeneity of mechanical characteristics. In the framework of this study, accuracy and convergence of the numerical solution by the finite element method (FEM) using the presented technique are determined. For this purpose, we used the SSS calculations of a human bone tissue (a fragment of the femur).

The selection of DS and its analysis are nonessential, but they are caused by important factors: heterogeneity of the bone material, individuality of its geometry, as well as high technology and quality of CT scanning in medicine. Bone tissue is well studied in practice, which makes it possible to reasonably consider the correctness of its mathematical simulation.

The first study uses parallelepiped specimens cut from a fragment of a human femur (Fig. 4*a*). The results of the study are shown in Fig. 4*b* as proof of accuracy and convergence of the FEM numerical solution with respect to the full-scale experiment data [9, 10].



a)



b)

Fig. 4. Dimensions and orientation of real samples (*a*); graph of convergence of normal stress in the center of samples (*b*), longitudinally (1), circumferentially (2) and radially (3)

The results show that to achieve the desired accuracy of the FEM numerical solution, a FE mesh with a density of three or more finite elements per 1 mm is required [11]. It is also obvious that the heterogeneity property of the DS material mechanical characteristics can be reflected by a set of finite elements with their own elastic moduli and the isotropic structure of the material.

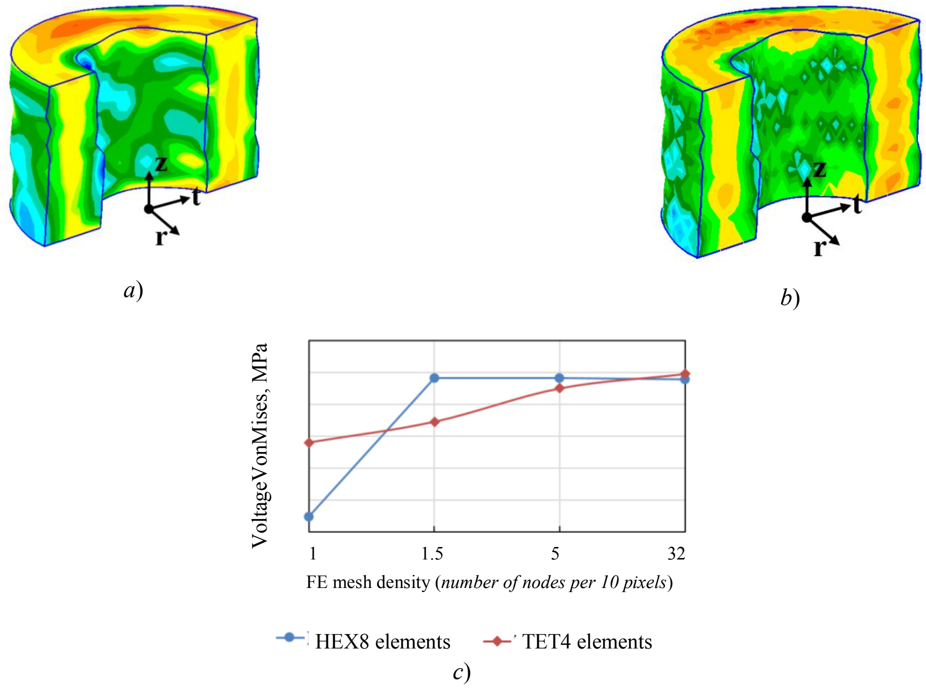
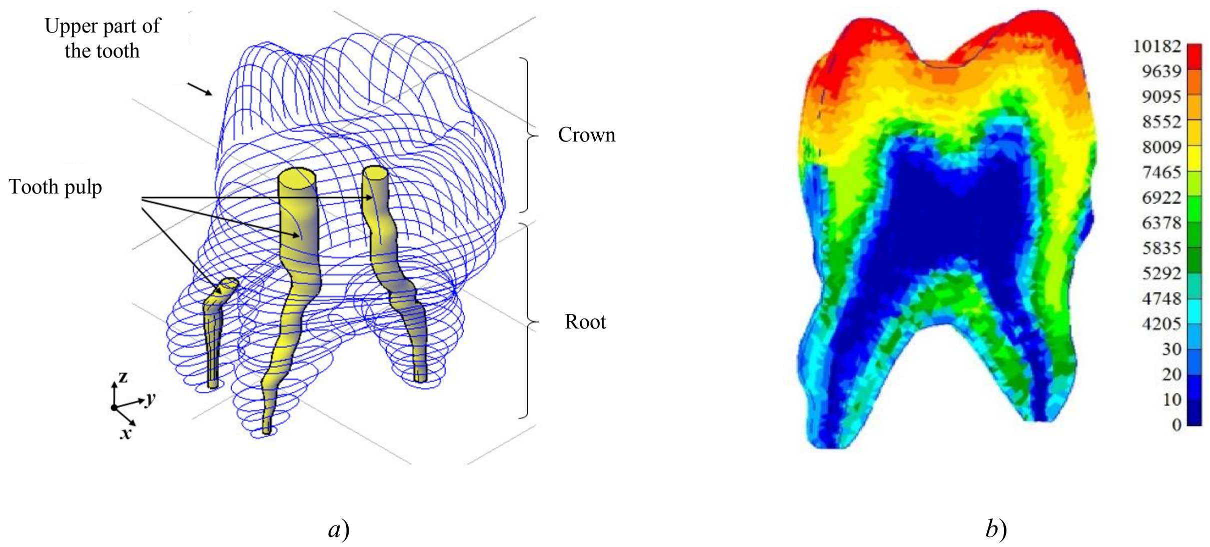


Fig. 5. SSS analysis result using HEX (*a)* and TET (*b*) type finite elements; graph of convergence results (*c*)

To study the applicability of two different types of solid FE (hexahedron and tetrahedron), an additional study was conducted using incompatible shape functions (see Fig. 5) [12]. The results show that hexahedron-type FE has the best indicators in terms of accuracy and convergence of results, as well as in the resource costs.

3. Modeling of real deformable solids. The technology presented is applied to real objects. For this purpose, the SSS of the FE of tooth setups with a defect and a sealant made of composite material was constructed and analyzed. One model presents a defect in the form of a carious region (cavity) in the upper part of the enamel. In the second version of the FE model, this area is filled with a sealant made of composite material. Both models are built considering heterogeneity of the material mechanical characteristics and an individual geometry.

A wireframe model of a human tooth, shown in Fig. 6*a*, is based on the scan results [13, 14]. A change in the material mechanical characteristics in the solid FE model (Fig. 6*b*) is simulated in a special program [13, 14]. Input data: results of scanning and field testing.



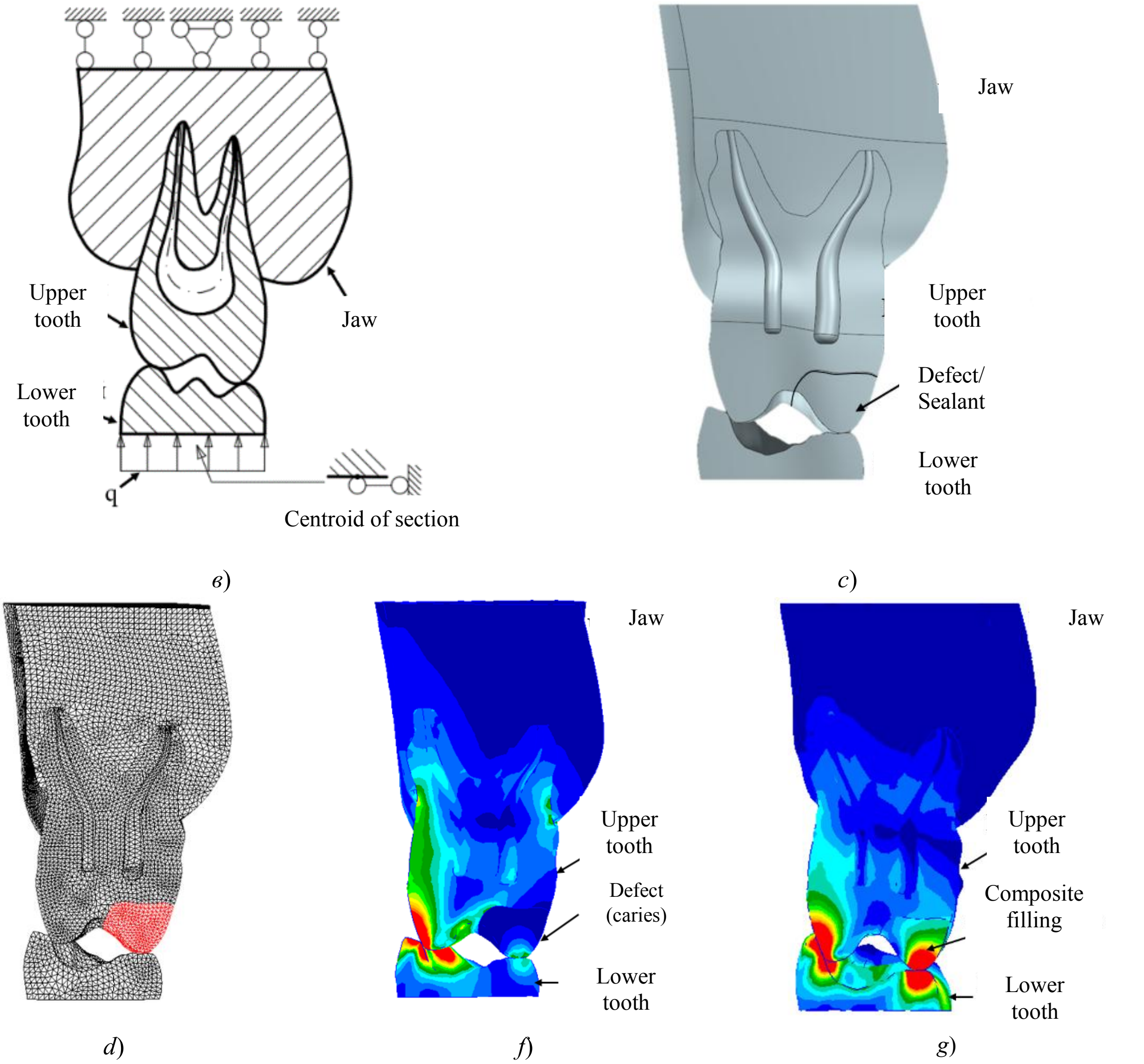


Fig. 6. Construction and analysis of FE models of a human tooth considering heterogeneity of material mechanical characteristics: *a*) wireframe model; *b*) change in elasticity tooth modulus in FE solid model; *c*) design scheme; *d*) solid geometric model; *e*) FE mesh generation; *f*) SSS analysis result of FE model of tooth with simulated defect; *g*) SSS analysis result of FE model of tooth with simulated composite fillings

The design scheme is presented in Fig. 6*c*. A defect and a composite filling are modeled on the upper tooth (see Fig. 6*d* and 6*e*).

The analysis result of the FE model with a defect (see Fig. 6*f*) shows that the carious part of the tooth does not absorb the load. That is, a healthy part of the tooth has an additional load, and the probability of decay increases. The analysis result of the second FE model, after filling the caries area with a sealant made of composite material (see Fig. 6*g*), shows that the tooth almost completely restores its functional capacities since the stress pattern is identical to the picture obtained for a healthy tooth [2].

Fig. 6*g* shows that stress maxima are observed at the contact points on the tops of the dental tubercles. A higher load is picked up by the area of enamel and dentin. The inner part of the tooth is less stressed. This result is compared to the calculation [2]. An average value of the mechanical characteristics of enamel and dentin is used. Heterogeneity of the structure of the tooth material is not taken into account. The comparison shows a more uniform stress distribution in the tooth body when modeling the distribution heterogeneity of its mechanical characteristics.

Discussion and Conclusions. The study results validate the accuracy and reliability of the presented method of FE modeling based on scanning real DS considering heterogeneity of the material mechanical characteristics.

The presented complex of mathematical methods for modeling the interpretation of CT scanning bitmaps allows the study of any complex structures of real DS. The results of such simulation are used to construct FE models considering heterogeneity of the mechanical characteristics of the material.

The developed mathematical modeling technique can be applied for any physical scanning principles (X-ray, ultrasound, laser, etc.) and for any types of materials if the data received is a digital (raster) image.

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Submitted 25.03.2019
Scheduled in the issue 17.06.2019

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