

Modified bone cement microstructure numeric simulation

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Materials

ABSTRACT

Purpose: The paper aimed at determining the strength of modified bone cement microstructure. Modification with aqueous hormone solution stimulates the growth of bone at a hip-joint endoprosthesis implantation site.

Design/methodology/approach: In the first place, microstructure of modified cements was examined. This examination was a basis for statistical description of porosity obtained as a result of modification. Statistical data were used to create microstructure models in a programme being in agreement with FEM technique. Simulations were carried out on structures of 2 types of pores, i.e. those containing water and empty ones.

Findings: Modification with aqueous solutions of modifying agents affects the structure and properties of bone cements. This is caused by formation of pores filled with aqueous solutions of modifying agents. This type of porosity decreases mechanical properties less than air-filled pores.

Research limitations/implications: Numerical simulation of the stress and displacement pattern in juncture microstructure should be expanded with a simulation of bone-cement-implant system operation, which will allow estimation of an optimum value of modifying agent admixture, i.e. a value enabling the improvement of juncture biocompatibility not lowering at the same time its mechanical properties below a level set up in standard specifications.

Practical implications: Microstructure simulations performed confirmed a manner of modified cement cracking observed on fractures. They showed formation of pore agglomerations where concentrating stresses may bring about the appearance of dangerous micro-fractures.

Originality/value: Cement modification with aqueous solution and examination of the effect of admixture on microstructure mechanical properties.

Keywords: Bone cement modification; Implants; FEM analysis; Microstructure assessment

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1. Introduction

Increase of the interest of many laboratories worldwide in research and development of new material technologies for this field generates a considerable inflow of scientific information.

From the point of view of bonding engineering, a problem of connecting biomaterials with a living tissue increases together

with their growing assortment. Not only new materials with specific properties but also diversified tolerance of organism to their presence constitute a problem.

A specific case of using the bonding techniques in medicine is application of cement bonds in hip, knee and shoulder joint alloplasty as well as in plastic and reconstructive surgery. The features of bone cement connections are, in their whole substance,

qualitatively similar to those of bonded joints used in construction of machines, mechanisms and tools or in electronic systems and, from the side of macro- and microstructural, mechanical and corrosive properties, they should be considered as binding materials using bonding engineering criteria expanded with requirements referring to biomedical properties.

An interesting example of using the mechanical properties of bio-bonds is implantation of human hip joint by means of bone cements. Bone cements based on polymethyl methacrylate (PMMA) belong to a group of self-polymerising acrylic resin materials. They have been implemented into clinical practice in the mid 50s for fixing joint endoprostheses and belong at present to most frequently used ones in treatment of osteoarticular and muscular system diseases and injuries.

Human hip joint is an example of spheroid acetabular joint characterised by an extensive scale of movements. Hip joint belongs to most exploited carrying joints in human motor organ [1].

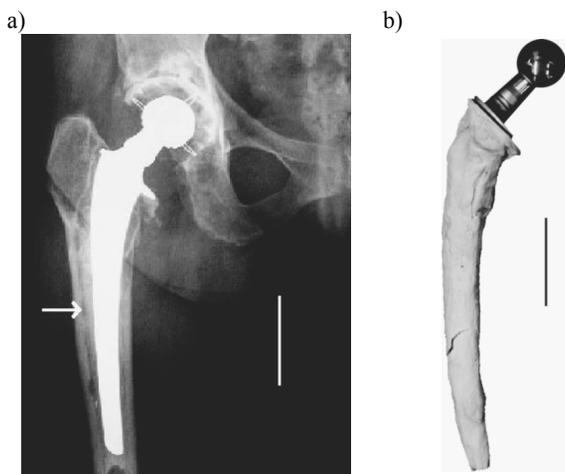


Fig. 1. Fixing of hip-joint endoprosthesis (markers corresponds to a length of 5 cm): a) radiographic picture of endoprosthesis in patient's body (frontal view); an arrow shows a loosening site, b) exemplary endoprosthesis after removal from patient's body (cement is still strongly clinging to prosthesis) [2]

Hip joint, having a considerable importance for the mechanics of human movement, is commonly exposed to pathological changes and injuries. In severe degenerative lesions or after femoral neck fractures, it is necessary to implant an artificial part or the whole joint in place of the natural one [3].

Appropriate construction of endoprosthesis should ensure a proper joint movement range, load transfer, overload capacity, vibration damping, bone mass stimulation and abrasion resistance as well as a possibility of carrying out a simple surgical operation. In order to fulfil these requirements, an appropriate geometry and type of implantation material should be chosen. The stress pattern in a juncture between a bone and an implant is determined by relations between their elastic properties. Static and fatigue strengths affect the size of transferred stresses and overload capacity whereas surface condition and its physical and chemical features determine the nature and the strength of juncture at the border of bone-implant phases [4, 5, 6].

Even though implantology gives possibilities of replacing damaged anatomical structures, it restores lost functions only for a certain period of time. A reason of that is a wear and tear of artificial joints, which leads with time to a repeated failure of function [7, 8].

After operations of joint alloplasty with the use of bone cement, a rather high percentage of cases with prosthesis functionality loss is observed caused by inflammatory and degenerative changes, bone destruction and aseptic loosening (Fig. 1). Therefore, research works are being accomplished aiming at improvement of parameters which characterise biofunctionality of implants. Further directions of development are being conditioned by permanently growing number of performed alloplasties, searching for new solutions in dangerous revision surgeries and economic reasons.

Application of developments from different areas of technical sciences is more and more frequently helpful or simply indispensable in everyday clinical practice, while implantology is one of the fields of medicine in which theoretical and experimental methods of materials science, including mechanics of materials, are particularly useful. This is because the prediction of consequences resulting from introduction of foreign bodies into human organism - like implants - requires knowledge of the effect of their biological and material properties on internal environment. Biological response of organism on graft insertion depends, among others, on their geometrical features, mechanical properties of components and biomechanical systems created this way and in particular on the stress pattern [1, 9, 10].

Exploitation of biocompatible cement junctures is frequently connected with complications induced by reactions of unreacted toxic components, thermal damages and infections. They lead to formation of the phenomenon of aseptic loosening of implants, which is a concern of a substantial number of research works accomplished so far. Implant loosening prevention is being accomplished in many ways. One of them is cement modification [11, 12].

Bone cements are modified with many agents that improve their operational properties, with a modifying agent participating in polymerisation reaction or being inactive. Addition of reactive modifying agents, apart from affecting strength properties, can also decrease the intensity of heat released during mixture hardening [13] through extension of reaction time or reduction of the amount of toxic MMA monomer being liberated into human organism after cement hardening [9].

Gentamicin-containing cements used so far show that within a certain time interval a drug is released from them into environment. Part of the authors is of the opinion that gentamicin release takes place by diffusion of compounds through polymer matrix or capillary through empty spaces inside it. Nevertheless, a considerable part of scientists examining the phenomenon of drug release from bone cements think that it strongly depends on surface roughness [13].

Until now, the phenomenon of gentamicin release has been closely examined. When comparing popular cements containing gentamicin used at present, one may conclude that release rate depends for the most part on such parameters as cement surface smoothness, porosity and wettability. These cements can be also modified with substances improving drug release rate [14, 15].

Results of the above-mentioned research works prove that gentamicin release from bone cements depends mainly on surface smoothness and porosity.

The kinetics of drug release from a cement prosthesis proceeds in two stages. Immediately after implantation, an initial release takes place which is fast and sharp. This release is connected with a large concentration of drug in the external layer brought into contact with external environment of filling. Initial release lasts about 40-50 hours.

After the first stage, a slow release of drug from prosthesis takes place. This stage is characterised by significantly smaller intensity and lasts very long. Cases are known of finding gentamicin traces in the proximity of prosthesis after 5 years.

The theme of using bone cements is very extensive and therefore it covers many areas where number of research works is insufficient to describe a full and complete solution of the problem of biomaterials connecting.

Aspects of bone cement modification with reactive and inactive admixtures in the context of a structure change affecting mechanical properties to the highest degree are a subject of significantly smaller number of analyses and surely require a certain extension.

These changes refer, among others, to increasing the porosity of admixture filled with incompressible aqueous solution and the smoothness and roughness of cement bond surface and decreasing the tensile and bending strength.

Data referring to the porous structure of cement bond and its effect on mechanical properties of modified bone cements published in literature are very fragmentary and cannot be a basis for detailed description of the problem.

Numerical simulation of cement bond described in the paper is to give a picture of the effect of modification of cement with aqueous solution on the stress and displacement pattern in microstructure of material.

2. Materials

The examined bond is bone cement which has been modified with a solution of salmon calcitonin CALCITONIN 100.

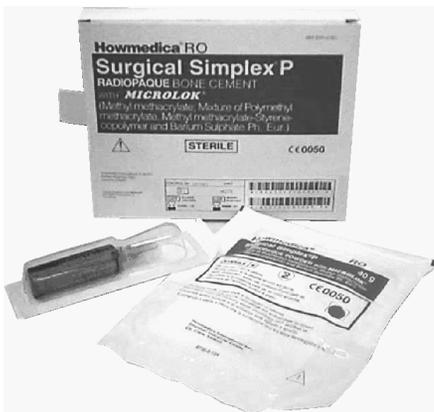


Fig. 2. Bone cement Surgical Simplex® P. View of the package containing a liquid monomer (glass vial) and powder (plastic bag)

Samples were made of bone cement Surgical Simplex® P (Howmedica Osteonics, Mahwah, NJ, USA). It is one of the cements most frequently used in hip-joint alloplasties (Fig. 2). It was prepared by mixing two components. First of them is a liquid solution of monomer with a characteristic acrylic smell. The second component of cement is a powder consisting mainly of filler and polymerisation initiator.

As a preparation consisting synthetic salmon calcitonin $C_{145}H_{240}N_{44}O_{48}S_2$, a generally available product under the brand name Calcitonin 100 was applied (Fig. 3). This preparation is frequently used in clinical practice.



Fig. 3. The preparation Calcitonin 100. Package containing 5 glass vial of 1 ml preparation

A larger part of the preparation (99.065% weight) is water therefore only the size of aqueous admixture [addition] and its effect on cement porosity should be taken into consideration when examining mechanical properties.

3. Porosity examination

In order to verify porosity analyses by the weight method and thoroughly learn the internal structure of modified cement, the image analysis method was applied. The image analysis allows description of pore morphology with statistical parameters, which made numerical simulation of the effect of porosity on cement structure possible in the further part of research work. Such a simulation will be then based on the real structure of porous cement bond.

During tests, total cement porosity was adopted to be a value characterizing the obtained cement. Also graphic interpretation of the porosity pattern was presented in the form of frequency distribution (frequency table) and relative abundance histogram.

Microphotographs taken on sample transverse micro-sections with the application of scanning electron microscope JOEL JSM-6100 were analyzed. Tests were carried out in three representative areas of $160 \times 120 \mu m$ for modified cement samples (Fig. 4).

Exemplary results of the statistical analysis of porosity on a transverse micro-section of sample with porosity of 8.3% are presented below (Table 1, Table 2 and Fig. 5).

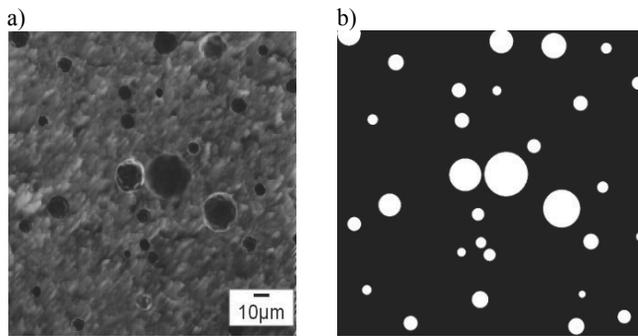


Fig. 4. Measured microsection of sample with porosity 8.3% a) photography of microsection; b) binary representation

Table 1.

Pores diameter (σ [μm]) in measured area of sample with porosity 8.3%

No	σ								
1	2.2	7	6.2	13	7.2	19	11.4	25	17.2
2	3.5	8	6.3	14	7.8	20	12.4	26	17.5
3	3.5	9	6.4	15	8.2	21	12.4	27	23.3
4	5.1	10	6.4	16	8.4	22	13.5	28	24.3
5	5.2	11	6.9	17	9.2	23	15.4		
6	6.2	12	6.9	18	9.4	24	16.4		

Table 2.

Pores frequency table for class number $k=6$ in measured area of sample with porosity 8.3%

σ range	Amount	Cumulative Amount	Percent	Cumulative Percent
$0.01880 < x \leq 4.39680$	3	3	10.7143	10.7143
$4.39680 < x \leq 8.81240$	13	16	46.4286	57.1429
$8.81240 < x \leq 13.2280$	5	21	17.8571	75
$13.2280 < x \leq 17.6436$	5	26	17.8571	92.8571
$17.6436 < x \leq 22.0592$	0	26	0	92.8571
$22.0592 < x \leq 26.4748$	2	28	7.14286	100
BD	0	28	0	100

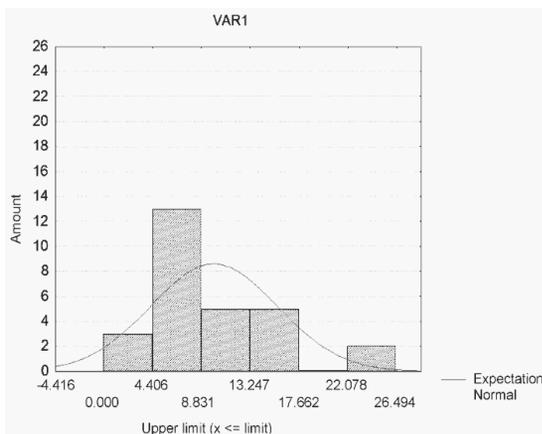


Fig. 5. Pores relative abundance histogram for class number $k=6$ in measured area of sample with porosity 8.3%

Determination of porosity using the image analysis confirmed the validity of results obtained earlier when measuring it with the weight method. When analysing representative areas, statistical features characterising the morphology of porous structure were estimated.

4. Microstructure examination

Microstructure examinations were carried out on sample fractures after mechanical tests using a scanning electron microscope JOEL JSM-6100.

The study aimed at determining the changes of cement structural and mechanical features affecting biofunctionality of bone-implant juncture and the cracking mechanism.

Exemplary microscopic photographs for samples with porosity of 8.3% and 13.4% are presented below (Figs. 6-9).

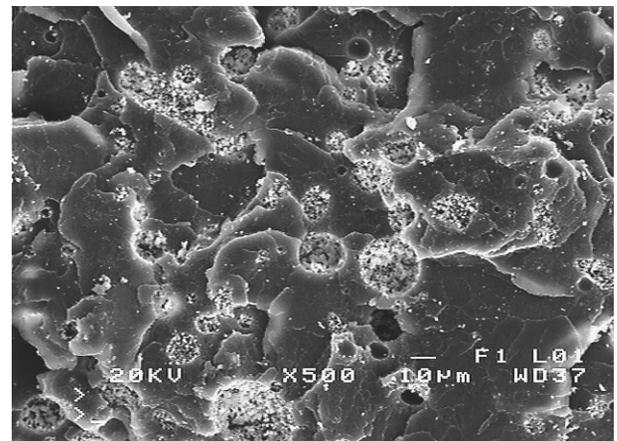


Fig. 6. Fracture microsection of sample with porosity 8.3%, magnification x500

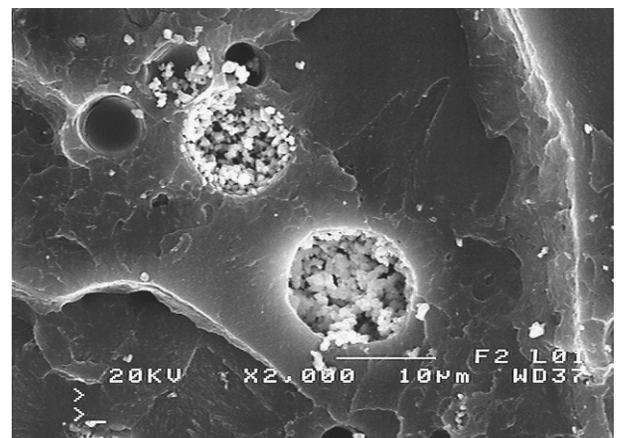


Fig. 7. Fracture microsection of sample with porosity 8.3%, magnification x2000

The analysed fractures have features of plastic fractures. Modified cements, with higher porosity, crack in places weakened by large clusters of pores. Therefore, formation of cracks takes place through resultant pores.

It can be seen on microphotographs with small magnification that pores are arranged irregularly and are of different sizes. This causes that finding a representative area in the structure is very difficult.

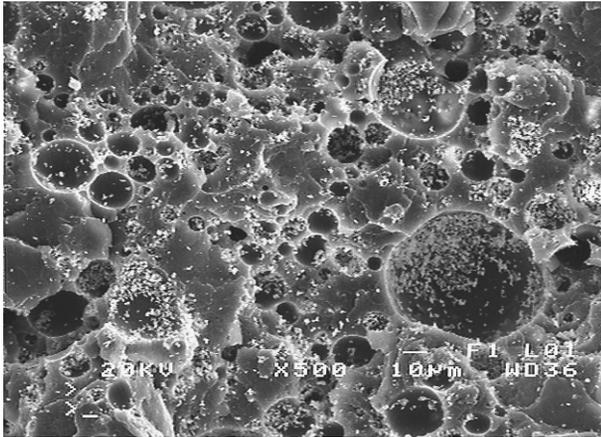


Fig. 8. Fracture microsection of sample with porosity 13.4%, magnification x500

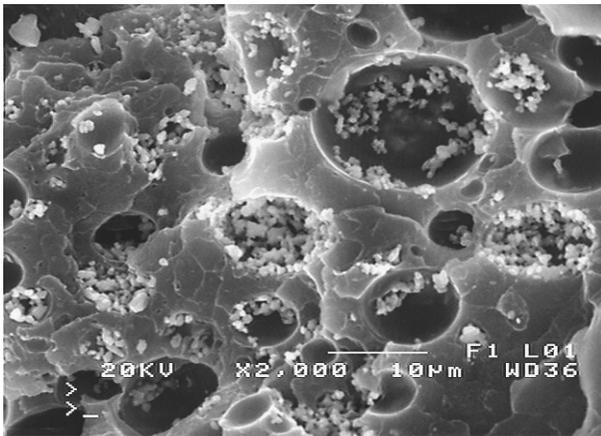


Fig. 9. Fracture microsection of sample with porosity 13.4%, magnification x2000

On microscopic photographs of cement fractures, crystal clusters of the solid components of aqueous calcitonin solution are also being observed in pores.

On the surface of fractures (cements), light inclusions in dark-grey polymer matrix are observed.

5. Numeric simulation of microstructure

Simulation aims at determining a difference in the stress pattern between the structure modified with aqueous calcitonin

solution (pores filled with water) and the porous structure with empty pores. Determination of differences in the intensity of stresses will allow evaluation of the effect of aqueous admixture on a change of the force system inside the material.

Geometric features of the model used in simulation were based on the longitudinal section of cylindrical sample for compression strength tests. Attention was focused on a square area of $190 \mu\text{m}^2$. Within this area, a structure corresponding with its statistical features to structures observed during microscopic examinations on transverse micro-sections was generated.

Porosity was determined by the following features:

- porosity;
- minimum pore diameter;
- maximum pore diameter;
- number of pores in a given category.

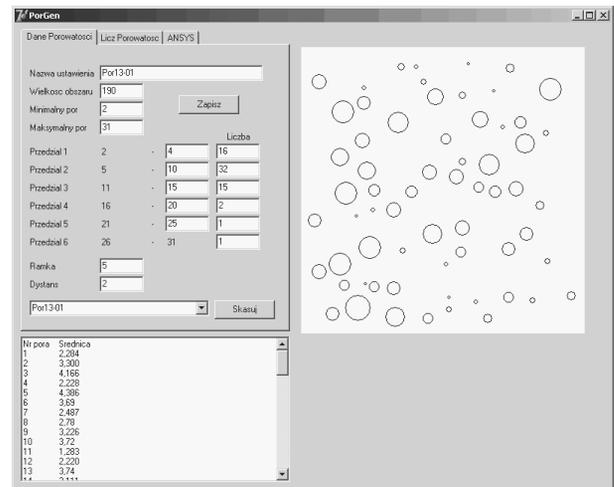


Fig. 10. Screenshot of ANSYS batch file generating application (porosity data input panel)

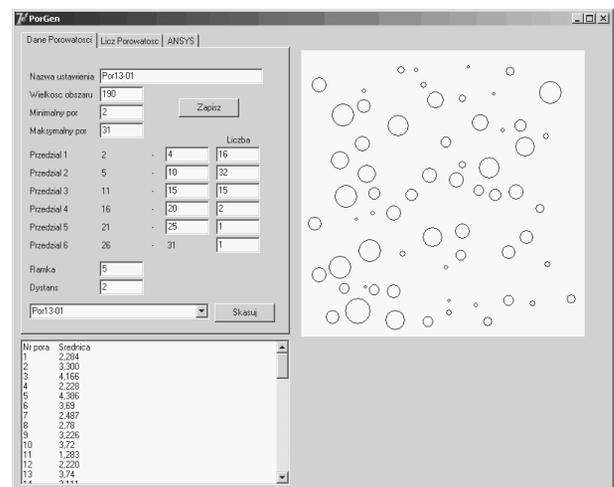


Fig. 11. Screenshot of ANSYS batch file generating application (generated structure parameters panel)

For structural analysis, an element of one type (PLANE82) was used, which is an element for two-dimensional analysis, i.e. a quadrilateral, eight-node element with interstitial lines of higher degree. This element has two degrees of freedom UX and UY. For this element, a thickness amounting to 0.05 mm was adopted.

Generation of the geometry with strictly determined parameters was obtained by an application created in person in the Object Pascal environment (Figs. 10-12). Based on assumed parameters, this programme generated a batch file for a programme being in agreement with ANSYS finite element method. Based on the batch file, ANSYS programme constructed in its environment the geometry for calculations, defined materials for respective areas and executed a structure division into finite element mesh (Fig. 13).

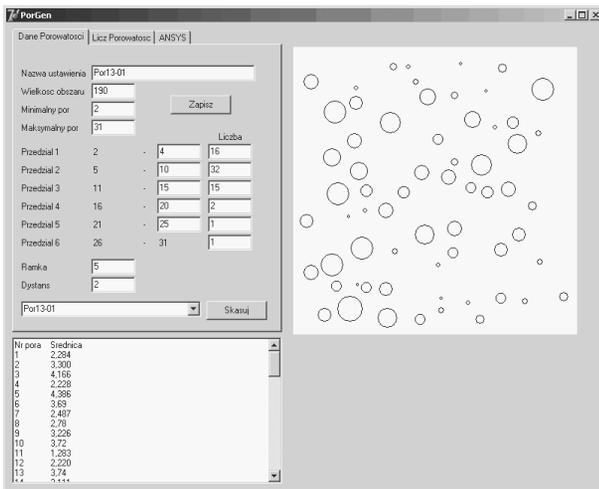


Fig. 12. Screenshot of ANSYS batch file generating application (batch file parameters panel)

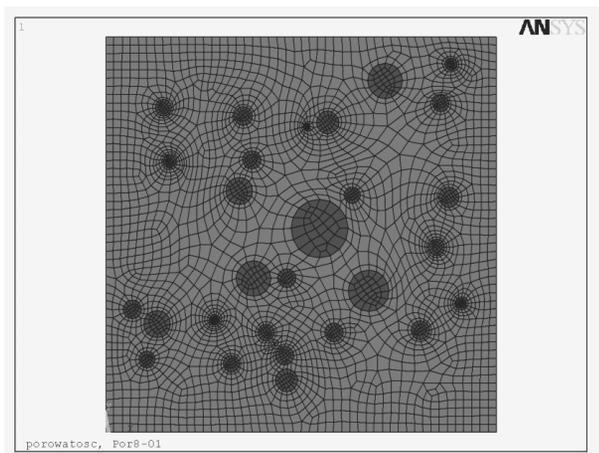


Fig. 13. Example of microstructure finite elements mesh

In the analysis, two types of material were taken into consideration. For materials outside the examined area, strength properties from mathematical models prepared during analyses

were adopted. Matrix properties in the examined area correspond to cement without admixtures. Features of the pore-filling material were chosen so that they copied water properties (incompressibility). For the matrix, a Young's modulus was adopted of a value of $3.9 \cdot 10^3$ [N/mm²], while for the pores of $1 \cdot 10^8$ [N/mm²]. In both cases, the Poisson's ratio ν amounted to 0.3.

The model was loaded with pressure applied onto the top edge with a positive value when compressing and a negative one when stretching. The generated stress state was within the elastic range. The produced model was fastened in a base, depriving it of all degrees of freedom.

Variants were tested in which static compression and tension of porous structure containing water and with no water was simulated.

In total, 6 generated models were examined being different in porosity, with 3 models for structures having the source porosity of 8.3% and 13.4% each. These models were loaded with tensile and compressive forces for 2 variants: pores filled with air (empty pores) and pores filled with water.

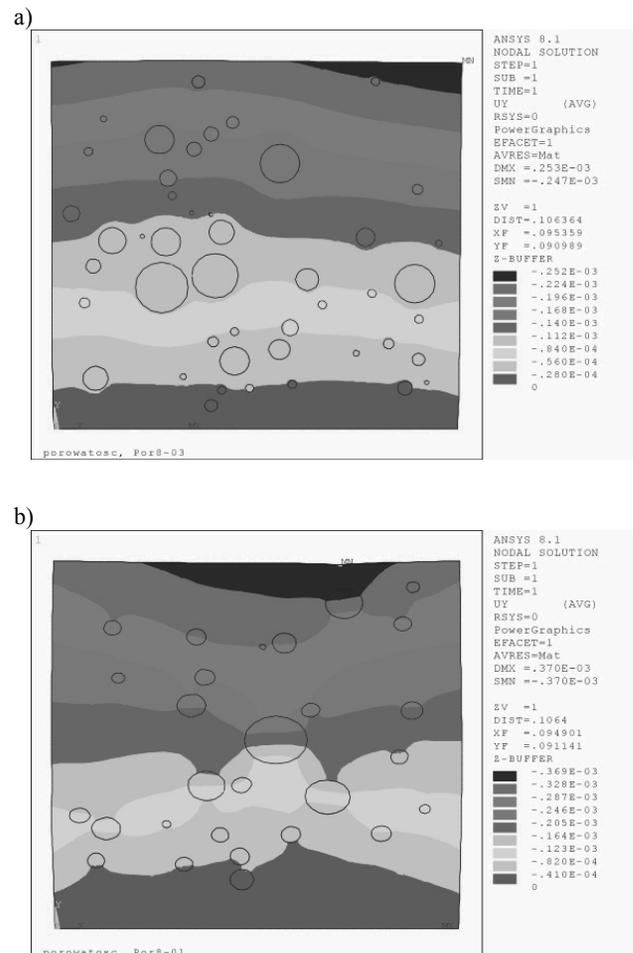


Fig. 14. Y axis strain for compressed microstructure with pores filled with: a) water, b) air

Earlier results of the statistical description of porosity obtained by transverse micro-section image analysis method were applied.

Sample deformations strictly depend on the number, size differentiation and arrangement of pores as well as on the type of material filling them (Fig. 14).

Deformations in samples with empty pores are larger and more diversified than in similar ones with filled pores (Fig. 15). The degree of differentiation of the above-mentioned features depends on pore segregation. The segregation phenomenon is observed in samples in which clear pore clusters are found. Displacement diagrams show largest deformations and largest differentiation between samples with empty pores and those with filled ones with growing pore segregation.

However, no significant differences in deformations were found together with the increase of porosity in the examined areas. A sample in which the number of pores is as twice higher as in other ones for porosity of 13.4% is an exception (Table 3).

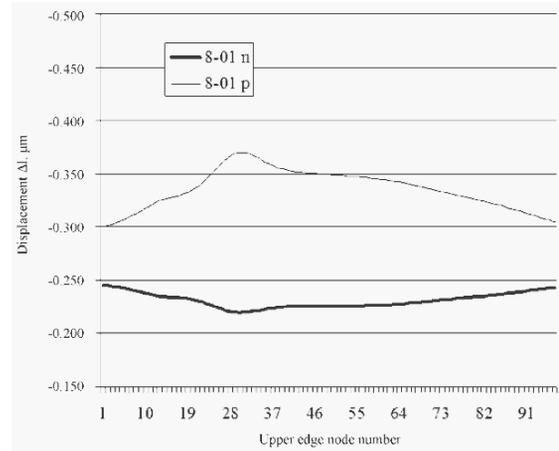


Fig. 15. Displacement upper edge of compressed microstructure: n - pores filled with water, p - pores filled with air

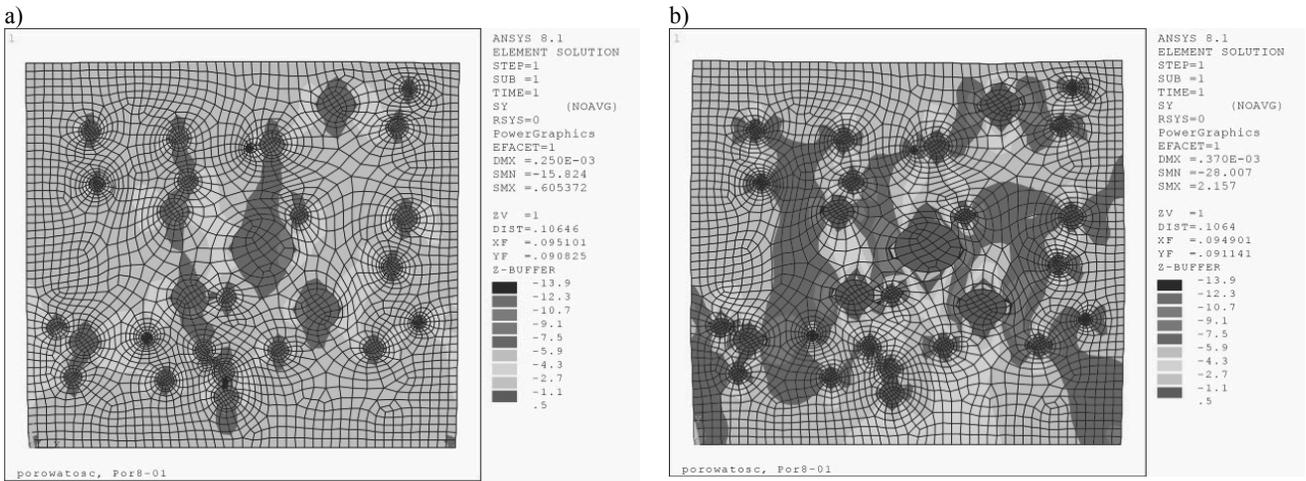


Fig. 16. Y axis stress for compressed microstructure with pores filled with: a) water, b) air

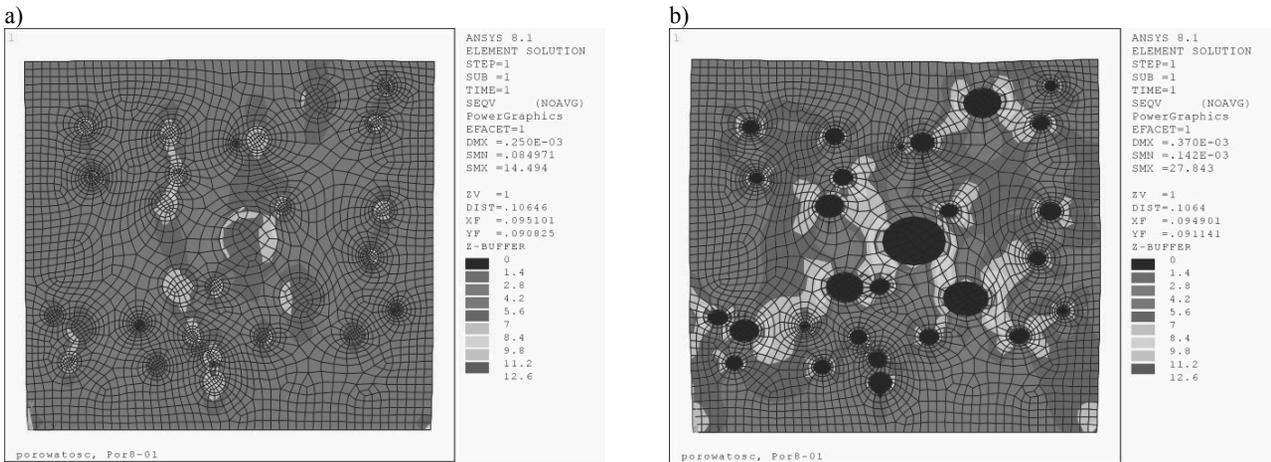


Fig. 17. Reduced stress for compressed microstructure with pores filled with: a) water, b) air

Table 3.
Result of deformation ϵ measurement

Porosity [%]	Displacement μm		Diff. [%]
	Water pores	Air pores	
8.3	-0.336	-0.231	31.1
8.3	-0.331	-0.232	29.9
8.3	-0.346	-0.227	34.3
13.4	-0.368	-0.220	40.3
13.4	-0.375	-0.218	42.1
13.4	-0.419	-0.206	50.8

Stresses increase slightly together with an increase of porosity, just as deformations. The increase of stresses together with porosity is larger in samples with empty pores (Fig. 16). The pattern of stresses on cross-section strictly depends on the arrangement of pores to each other. Stresses concentrate in pore clusters, reaching maximum values in the material delimiting two adjacent pores. The smaller the space between such pores, the larger is the stress (Fig. 17). The above-mentioned observations explain results of the microscopic examination of micro-sections in which a tendency was observed towards formation of cracks in the areas between adjacent pores.

6. Conclusions

Porosity examination with the weight methods was verified by means of metallographic analyses on transverse micro-sections. No significant differences were found in determining the porosity with these two methods. Porosity increases together with an increase of the content of aqueous solution of admixture in cement structure. Initially, pores are arranged evenly but then, with large porosity, they cluster together in agglomerations. This causes irregularity in bond properties. With high porosity values, it comes to connection of pores in developing pore agglomerations. Cracks in modified samples with porosity of 8.3% and 13.4% are formed in a thin polymer matrix between pores. Inside pores, crystal clusters of the solid components of Calcitonin 100 solution are observed.

Results of the microscopic observations of micro-sections of the representative areas of modified cement structures are expressed in figures. For samples with porosity of 8.3%, the number of pores ranged within the limit of 28-46 for an area of $160 \times 120 \mu\text{m}$. With higher porosity, the number of pores for the same area size was from 67 to 143. The larger the porosity, the larger is the scattering of results.

Statistical description of the photographs of metallographic micro-sections allowed also using the data from real structure analyses for generation of artificial structures which will be possible to be used in numerical calculations.

Simulation of porous structure loading aimed at depicting the stress and deformation pattern according to structure morphology. The prepared samples were loaded in two variants by means of an application generating structures corresponding to real structure parameters compiled by the author of this paper. Sample with empty pores showed static loading of modified cement in which pores were filled with air. The second variant is the same samples containing filled pores. Material filling the pores was defined as

undeformable so as to simulate a resistance of incompressible water being found in pores at dynamic loading.

On the prepared deformation diagrams, there are two curves describing a maximum displacement with empty pores as well as a minimum displacement when water in filled pores offers a resistance at dynamic compression. Difference between two variants is about 30% for porosity of 8.3% and 45% for porosity of 13.4% in favour of the variant with filled pores.

Similar is the situation with stresses towards the Y axis and reduced stresses which are significantly smaller in the variant with filled pores. Stresses concentrate in pore agglomerations, reaching maximum values in thin walls between adjacent pores. Porosity results in pore segregation and increases internal stresses in the polymer matrix.

Modification with aqueous solutions of modifying agents affects the structure and properties of bone cements, mainly in result of creation of pores filled with aqueous solutions of modifying agents. The filling of pores with incompressible medium, with negligible compressibility when compared to air under operating conditions, causes that this type of porosity decreases mechanical properties to a lesser extent than pores filled with air.

Aqueous admixture increasing the porosity causes an increase in local stresses in cement. Together with increasing porosity, a risk of development of pore agglomerations in which stresses are being concentrated may bring about the appearance of micro-cracks. These cracks are a potential threat for the bond since during use they may expand deteriorating the operation of implant-cement-bone system.

Numerical simulation of the pattern of stresses and displacements in juncture microstructure should be expanded with a simulation of the operation of bone-cement-implant system, which will allow estimation of an optimum value of modifying agent admixture, i.e. a value enabling the improvement of juncture biocompatibility not lowering at the same time its mechanical properties below a level set up in standard specifications.

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