Effect of Silver Nanoparticles Incorporation in Dental Resins on Stress Distribution

Finite element analysis

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To induce antibacterial properties, more attention has been paid to the incorporation of silver nanoparticles (AgNps) into acrylic resins. This method aims to avoid or at least to decrease the microbial colonization over dental materials, increasing oral health levels. Even all researchers agree on the antibacterial effect of AgNps, the influence on the mechanical properties is still controversy. A mathematical model created through Finite Element Method was used to compare the tensions induced by different concentrations of nanoparticles into the acrylic resin. With Finite Element Analysis can be avoided large number of experimental specimens. In our study we aim to evaluate the effect of 80 nm AgNps incorporation on the stress distribution in dental acrylic resins. Our results showed that the best concentration of the 80 nm AgNps, that not affect the mechanical characteristics of the material is 5%.

Keywords: silver nanoparticles, acrylic dental resins, finite element analysis

Acrylic dental resins are commonly used in dentistry for different purposes such as partial and complete denture, epithesis, orthodontic functional appliances, anti-snoring or bruxism mouth guard, due to their advantages: good physical properties, sufficient strength, low water sorption, low solubility. However, a series of disadvantages have also been reported: poor mechanical properties, high coefficient of thermal expansion, low modulus of elasticity and mucosal irritation, caused by the release of methyl metacrylate or by the bacterial colonization. Over years, many attempts have been made to improve the mechanical properties of acrylic resins in three directions: the development of alternative materials [1-3], the chemical modification by the addition of various polymers [4-6] and the reinforcement of PMMA with other materials, such as carbon fibers, glass fibers, metallic inserts. Recently, to induce antibacterial properties, more attention has been paid to the incorporation of silver nanoparticles (AgNps) into acrylic resins. AgNPs incorporation aims to avoid or at least to decrease the microbial colonization over dental materials, increasing oral health levels and improving life quality [7,8]. AgNps have been satisfactorily incorporated into polymers used as tissue conditioners and as denture base. The influence on the features of resins depends on the type of nanoparticles (size and shape), and concentration as well. AgNps have been added to resins due to their proved antimicrobial effects, but their influence on the mechanical properties is not completely elucidated. Even all researchers agree on the antibacterial effect of AgNps, the influence on the mechanical properties is still controversy. Some experts found that AgNPs incorporation within acrylic prosthesis material can improve its physical and mechanical properties [9], while there are also studies demonstrating negative effects on the resins features [10]. In our study we aim to investigate the distribution of tensions in a dental acrylic resin reinforced with AgNps, with 80 nm diameter, in four concentration: 5, 10, 15 and 20% weight percent. For revealing the stress field at the particle/matrix interface it was conducted a finite element analysis [11,12]. In dentistry, Finite Element Analysis has been used to simulate different dental structures and internal stresses in teeth and dental materials. Because of the large inherent variations in biological material properties and anatomy, mechanical testing involving biomaterials usually require a large number of samples [13].

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Experimental part

Materials and methods

To determine the tensions within a composite material consisting of silver nanoparticles and acrylic resin a FEM analyze was performed, using Autodesk soft (Autodesk AutoCAD 2014 and Autodesk Simulation Mechanical 2014). Designing the geometry of the resin is a complex procedure that requires a higher accuracy. In order to create the mathematical model it should be understood the physical behaviors of the composite material, predicted the performance and the behaviour of the design and identified the optimal concentration. The Finite Element Method is a computational technique which is dividing a model body into an equivalent system of many smaller units (finite elements) interconnected at nodal points. For the analysis we considered two hypotheses: assumptions related to the mechanical solicitation of the material and assumptions concerning the type of the tested material [14, 15].

Geometric characteristic determinations

We considered for this analyze an acrylic resin enriched with 80 nm AgNps, in several weight concentration: 5, 10, 15 and 20%. If the silver density is 10.49kg/dm^3 and the acrylic resin density is 1.51kg/dm^3 and considering an uniform distribution of silver nanoparticles into the resin, it is assumed that every nanoparticle is located in the center of a cube.

From geometric point of view, each nanoparticle is situated at an equal distance of one to the other, in three directions: two horizontal and one vertical. The results are summarized in table 1.

AgNps diameter [nm]	AgNps volume [nm^3]	AgNps weight [g]	Concentration [%]	Resin weigth [g]	Resin volume [nm^3]	Total volume [nm^3]	Side of the cube [nm]
80	268082,5	2,812·10-15	5	53.43·10^{-15}	35621025	35889107	329.85
			10	25.31·10^{-15}	16873117	17141199	257.84
			15	15.94·10^{-15}	10623814	10891897	221.67
			20	11.25·10^{-15}	7499163	7767245	198.04

Table 1
THE CUBE SIZE ACCORDING TO SILVER NANOPARTICLE DIMENSIONS

The solid model is transferred into a finite element analysis program, where a 3D mesh is being created, and subsequently the stress distribution analysis performed.

The finite element analysis consists in two steps [16]: modeling the structure /system and simulating factors acting on the system. For the analyze it is necessary to define: the geometric field of the problem, the elements to be used, the geometric properties of the elements, the element's connectivity and the physical constraints. A mathematical model is developed based on analysis of the data in relation to the phenomenon of interest and define the problem to be solved. Data for the theoretical modeling are established at this stage seeking answers to a minimum series of questions concerning synthesis of the geometric structure, synthesis of the material properties, synthesis of the support and of the loads acting on the system and the result to the FEM analysis [17].

Geometric structure realization

The geometric model is based on a cube, with the side corresponding to the diameter of the nanoparticle (table 1), centered in the cube. These structural units were arranged as it follows: four on the length, three for the width and four for the height, resulting in a final volume of 48 nanoparticles (fig.1). This arrangement was elected due to limitations on items number that can be used in finite element analysis, but also for the accuracy of the results. For the final results interpretation only the items located in the center of the structure will be taken into consideration.

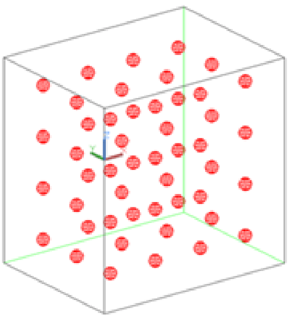

Fig. 1 Distribution of the AgNps into the acrylic resin

FEM analysis consist in a mesh realization by splitting a solid volume into finite elements, of parallelopipedic or tetrahedral shape. Each element behaves individually, with the same characteristics as the base material. Depending on the action applied on every element, a specific load or temperature will be supported, and will be transmited to the adjacent elements through nodes. For a better accuracy of the results a condition was imposed for the

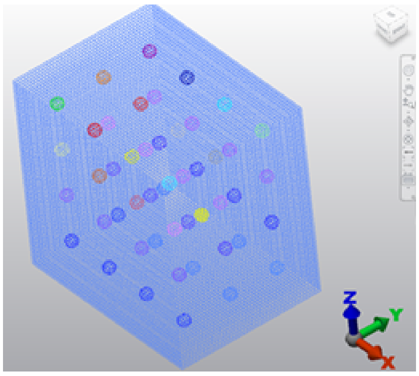

Fig. 2 The results of the meshing procedure

mesh realisation: the lenght between two nodes must be allways the same, according to the diameter of the silver nanoparticles; so, for a 80 nm diameter the chosen +length is 2 nm (fig. 2).

Synthesis of the material properties

The material used in the finite element analysis was a composite consisting in AgNps incorporated in the acrylic resin matrix. The material's properties used in the analysis were: the modulus of elasticity, Poisson's ratio, and density (table 2).

Synthesis of the support and of the loads acting on the system

The load acting on a volume element of the composite material (the cube with 48 AgNps) is based on several biomechanical aspects of the mandibular movements. The most important masticatory muscles are the masseter (on the external side of the lower jaw) and pterygoid muscles on the (internal sur face of the mandible). For the load application we considered the moment of the maximum force developed by the masseter and pterigoid muscles during mastication (total value 16000N.mm). On the volume element of the composite material a pressure of 8 MPa was applied to the upper surface (yellow) and constraints were applied on the lower surface (green) (fig. 3).

Results and discussions

Using finite element analysis we determined two main features: Von Mises stresses and volume element deformations. In order to visualise the stresses inside the volume element we used the option slice planes, which makes a section on a plane in the center of the volume element. Thus, it was established the section plane XZ (fig. 4).

Element	Modulus of elasticity [MPa]	Poisson's ratio	Density [kg/m^3]
Acrylic resin	2000	0.39	1.5
Silver	76000	0.37	10.491

Table 2
MATERIAL CHARACTERISTICS FOR EACH COMPONENT OF THE FINITE ELEMENT ANALYSIS

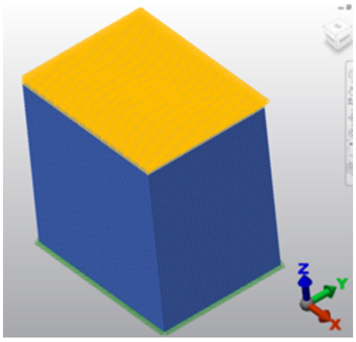

Fig. 3 Pressure application (yellow) and the support (green) to the volume element of the composite material

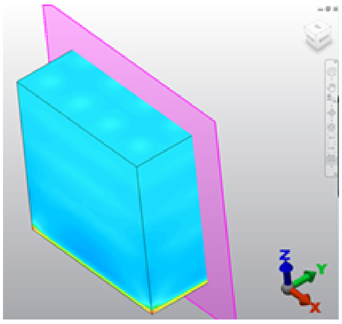

Fig. 4 The section plane XZ in the center of the volume element

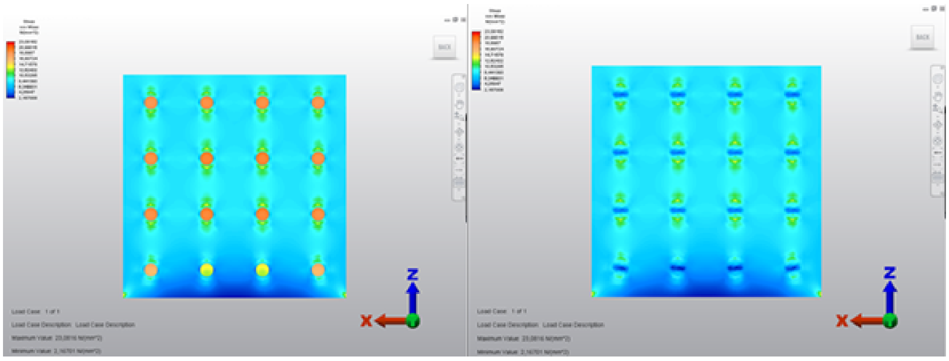

Fig. 5 Tension value in section XZ

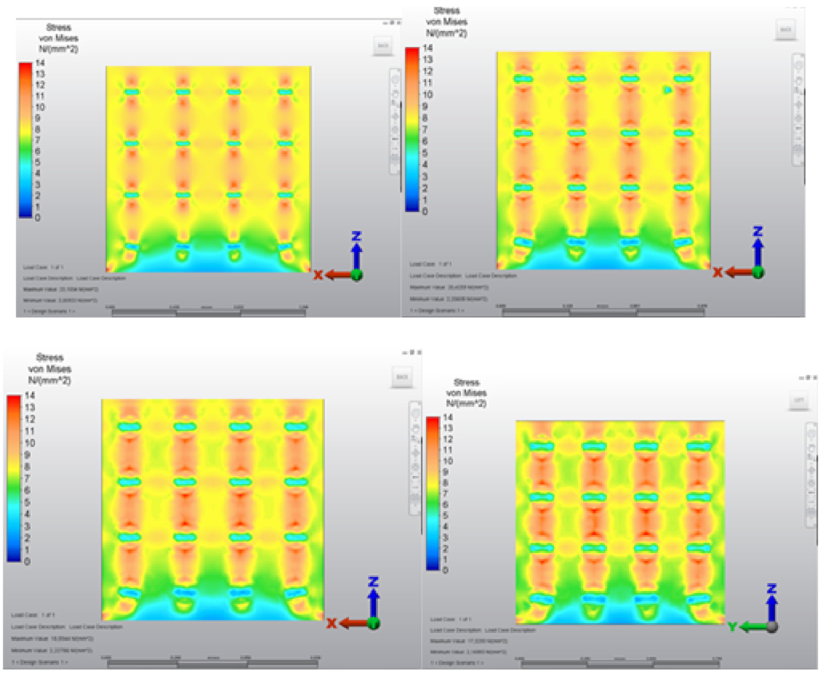

Fig. 6 The tensions distribution inside the reinforced resin with concentration 5%, 10%, 15% and 20% AgNps

Table 3

DETERMINATION OF THE NANOPARTICLE NUMBER PER VOLUME (mm³)

AgNps diameter [nm]	Concentration [%]	Total volume [nm³]	Number of nanoparticles/mm³
80	5	35889107	$1.33745\cdot10^{12}$
	10	17141199	$2.80027\cdot10^{12}$
	15	10891897	$4.40695\cdot10^{12}$
	20	7767245	$6.1798\cdot10^{12}$

In order not to affect the analysis results, this plan can be setted to zero visibility. The picture 5 shows two variants of the same section, one that reveals the silver nanoparticles and the other whith the nanoparticles setted to zero visibility.

Basically, it is interesting to analyse the stress that occurs in the acrylic resin. The maximum load into the acrylic resin is 14 Mpa, lower than the maximum load supported by the acrylic resin, which is 30 N / mm² [16].

Therefore, for all considered cases, the maximum load of 14MP will be imposed (in legend properties - as a maximum value visualized). So, it is possible to compare the difference between different values of loads, for each concentration. Picture 6 illustrates the stress distribution inside the acrylic resin, when the composite material contains 80nm AgNps, of 5, 10, 15 and 20% weight concentration (fig. 6).

Comparing the results of this analysis, it can be noticed that, although the maximum amount of tension around AgNps has the same value, in the central area, which is relevant for the analysis (on columns 2 and 3 between rows 2 and 3) the lowest stress was found at 5% concentration, while the highest value of the stress corresponds to 20% concentration A lower loading is generating a lower stress into the acrylic resin, especially for the fatigue strength of the material under dynamic conditions. Another important aspect is concerning the nanoparticle density per volume unit. Table 3 shows the number of the particles per mm³ data into the performed analysis.

Taking into consideration the results of table no 3 and in figure 5 it is obvious that the optimal AgNps concentration is 5%, from both biological and mechanical point of view.

Conclusions

AgNps incorporation aims to avoid or at least to decrease the microbial colonization of the acrylic dental resins In order to predict the optimal distribution and concentration of AgNps, we used a finite element analysis, revealing the stress field at the particle/matrix interface.

Our FEM study demonstrates that for the 80 nm AgNps, the best concentration, that does not affect the mechanical characteristics of the acrylic resin is 5%. According to the biological criterion a 10% concentration can be also used, because the stress inside the material being not significantly different in comparison to the situation registered for 5% concentration.

The FEM analisys should be accomplished by mechanical tests and in vivo experiments in order to sustain the final conclusions and to indicate a better antimicrobial material for the prosthodontic treatment.

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