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© O. Dolgov[1], O. Datsok[2], O. Naumenko[1]
[1] Dnipro University of Technology, Dnipro, Ukraine
[2] Kharkiv National University of Radio Electronics, Kharkiv, Ukraine

QUALIMETRIC ASSESSMENT OF RESTORATIVE DENTAL NANOCOMPOSITE MATERIALS

О.М. Долгов[1], https://orcid.org/0000-0003-3615-9032
О.М. Дацок[2], https://orcid.org/0000-0003-4489-3819
О.Г. Науменко[1] https://orcid.org/0000-0002-9532-1493
[1] Національний технічний університет «Дніпровська політехніка», Дніпро, Україна
[2] Харківський національний університет радіоелектроніки, Харків, Україна

КВАЛІМЕТРИЧНА ОЦІНКА РЕСТАВРАЦІЙНИХ СТОМАТОЛОГІЧНИХ НАНОКОМПОЗИЦІЙНИХ МАТЕРІАЛІВ

Purpose. To analyze the mechanical characteristics of dental materials in comparison with enamel and dentin properties of teeth and to develop a method for qualimetric assessment of the modern biomechanical restorative materials effectiveness use in minimally invasive dental practice.

The methods. For the restorative materials quantitative assessment, a method was proposed and substantiated, based on the concept of the average harmonic ratio of the elasticity modulus, strength, crack resistance and hardness of artificial materials to the corresponding natural enamel and dentin properties. The quality indicators of enamel and dentin are accepted as equal to one. Accordingly, the closer the quality indicator of the restoration material is to one, the closer it is to the characteristics of natural material according to the selected criterion, i.e., it is the best of the options considered.

Findings. The mechanical parameters of the five restorative composite materials were systematized and calculations of the proposed complex indicator of their quality reduced to the properties of tooth enamel and dentin were carried out. A comparative analysis of the results obtained confirms the conclusion that it is impossible to assess the overall quality of the materials studied based on a single mechanical characteristic. The calculations conducted confirm the possibility of applying the proposed methodology.

The originality. The dependencies established between the basic parameters used to evaluate the mechanical properties of dental nanocomposite materials (modulus of elasticity, strength, crack resistance, hardness) can be used to improve methods for qualimetric assessment of biomechanical materials. For qualimetric assessment of materials using the considered method, there are no fundamental restrictions on basic parameters increasing number.

Practical implementation. The results obtained from research into restorative composite materials based on a comprehensive quality indicator can contribute to a reliable practical assessment of existing and new dental materials to reduce risks and increase the effectiveness of their practical use.

Keywords: *minimally invasive dentistry, nanocomposite, biocompatibility, qualimetric assessment, photopolymer, material properties.*

Introduction. In 2022, the World Health Organization (WHO) published the Global Oral Health Report. It provides data profiles for 194 countries and presents a comprehensive picture of oral health worldwide [1]. In accordance with Report oral diseases are among the most common noncommunicable diseases worldwide, affecting an estimated 3,5 billion people.

Unfortunately, the number of such cases has been increasing over the years. Recently, bioactive dentistry, the main principle of which is the use of bioactive materials, has been playing an increasingly important role in solving this problem [2–5].

The quantitative assessment relevance of the restorative dental materials quality is due not only to the aggravation of dental diseases in people around the world problem, but also to the use of a large number of nanocomposites, which are not always safe and sometimes far from complying with the conditions of biocompatibility. Nanohybrid photopolymers in restorative minimally invasive dentistry play an increasing role and are gaining practical application as biomimetic materials due to the possibility of regulating mechanical, physicochemical and biological properties. These materials are analogues of natural tooth structures. The goal of modern dental restorative procedures using biomimetic materials is to return hard dental tissues to their full function, because they are able to imitate and restore natural dental biomechanics. Modern dentistry is increasingly moving away from traditional treatment methods, as more invasive, and uses biomimetic materials in combination with reliable adhesive systems to preserve the natural properties and structure of dental tissues. This approach leads to an increase in the period of operation of restorations and, to some extent, reduces the risk of complications.

The development of correct methods of qualimetric assessment along with the creation of new effective materials will further improve the quality of restorative dentistry.

As is known, the materials biocompatibility problem is associated with various aspects of their safe use, which depends on the nature of their interaction with the body tissues [6]. However, there are a large number of other factors that can negatively affect the reliable use of restorative materials. In this regard, it is necessary to know how resistant the materials are to the forces that arise during the act of chewing and occlusion, during shrinkage of the material, polymerization or expansion and compression of the material under thermal influences. Dental restoration may not be mechanically strong enough, which will lead to destruction or severe wear of the filling or prosthesis; this may be due to the wrong choice of restorative material, the properties of which do not meet the conditions of its clinical application. Thus, the study of the properties and comprehensive assessment of the quality of restorative dental materials, given their diversity, are very relevant.

The state of the issue and the research problem. It should be noted that currently there is no thoroughly substantiated criterion or scale by which it is possible to determine the best composite bone analogue. In [7], an index is proposed for assessing the quality of the material compared to the quality of natural bone. This index is based on the fact that the following properties are of great importance in assessing artificial materials that replace bone: 1) modulus of elasticity; 2) strength; 3) fracture toughness; 4) bioactivity.

According to these characteristics, for orthopedic materials, a quality index of their effectiveness in comparison with natural bone (cortical and cancellous):

$$I_q = \frac{K_{1c} \times I_b \times UTS}{E}, \qquad (1)$$

where K_{1c} – is fracture toughness; I_b – bioactivity index; E – the Young's modulus; UTS – ultimate tensile strength.

In our opinion, this approach has significant drawbacks:

1. The index is dimensional and thus depends on the system of units in which each parameter is measured.

2. The bioactivity scale, in itself, is conditional and, as a result, introduces an arbitrary character into the definition of the index.

3. The tensile strength is considered, although it is more expedient to take into account the compressive strength.

4. The modulus of elasticity appears in the denominator without justification, and not some other indicator.

5. A very important physical and mechanical property of the material – hardness – is not taken into account.

Since the enamel and dentin properties differ significantly, it is advisable to introduce parameters that are the ratio of the restoration material characteristics to the corresponding values, enamel and dentin. Thus, the quality assessment of dental composites is carried out in comparison with enamel and dentin separately. After determining these parameters, a complex quality indicator is proposed for consideration, in which not only mechanical, but also other characteristics may appear. For such an indicator, we will consider the harmonic mean of the above parameters.

The main part. According to the definition [8], the harmonic mean is considered as one of the averaging types, that is, a special case of the power mean with index −1. Thus, the harmonic mean H for n numbers $x_1, x_2, \ldots, x_n > 0$ can be written as

$$H = \frac{n}{\sum_1^n \frac{1}{x_n}}. \qquad (1)$$

In our case, the mechanical properties of photopolymers are considered, namely: modulus of elasticity, compressive strength, crack resistance and hardness. Then

$$n = 4, x_1 = \frac{E^m}{E^t}, x_2 = \frac{\sigma^m_{\max}}{\sigma^t_{\max}}, x_3 = \frac{HK^m}{HK^t}, x_4 = \frac{K^m_c}{K^t_c}, \qquad (3)$$

where E^m, $\sigma^m_{\max}$, HK^m, K^m_c – respectively, the modulus of elasticity, compressive strength, hardness and fracture toughness of the restoration material; E^t, $\sigma^t_{\max}$, HK^t, K^t_c – similar enamel or dentin characteristics.

As mentioned above, further analysis will be carried out in comparison with the characteristics of enamel and dentin, i.e. in Eq. (3) the numerator includes indicators for artificial material, and in the denominator – separately for enamel or dentin. The enamel and dentin quality indicators, thus, are equal to one. It is clear that the closer the quality indicator of the restoration material is to one, the closer it is to the characteristics of the natural material according to the selected criterion, and i.e. it is the best of the options considered.

It should be noted that the list of basic characteristics according to this method can be expanded. For example, tensile and bending strength, impact strength, etc. can be added to mechanical properties. It is possible to consider other properties that are not included in the list of mechanical ones, for example, roughness before and after simulated cleaning, etc. Adding other parameters does not limit the use of the proposed approach, provided that the initial data are correctly systematized.

When conducting a comparative analysis of mechanical properties, it is also necessary to consider the effect of light radiation on the quality of dental composite polymerization. The operating modes of polymer lamps, which specialists can use when performing restoration work for certain composites and clinical scenarios, affect the quality of polymerization and the durability of dental composites.

When comparing light-curing modes, the traditional polymerization mode shows higher hardness indicators [9]. The normal mode provides an intensity of 550 mW/cm^2 and a recommended curing time of 20 seconds, giving a total energy of 11000 J/cm^2. High-intensity mode provides an intensity of 1160 mW/cm^2 and a manufacturer-recommended minimum curing time of 10 seconds, resulting in a total energy of 11600 J/cm^2.

The total energy is almost the same for both light curing times. But the lower hardness for the high-intensity mode may be due to the following factors:

– light intensity dispersion, as the standardized distance equalized the intensity to the level of normal mode; therefore, the light curing time was different for normal and high intensity modes;

– high-intensity curing accelerates polymer formation, creating shorter chains, which in turn reduces the modulus of elasticity and hardness of the restorative dental composite materials.

It is important to choose a light-curing device and allow sufficient time for satisfactory polymerization of the hybrid dental composite materials, especially for restorations involving deep cavities.

To quantitatively assess the quality of dental materials by mechanical properties according to the proposed methodology, we will consider the characteristics of photopolymers from leading manufacturers of dental materials: Vittra APS (FGM), Z350 XT (3M ESPE), Tetric N-Ceram (Ivoclar Vivadent), Estelite Quick (Tokuyama), Charisma Diamond (Heraeus Kulzer). The basic parameters will be considered as the modulus of elasticity, compressive strength, fracture toughness (crack resistance) and Knoop hardness.

If the determination of the initial data for artificial materials, based on the literature, can be carried out relatively easily, then the systematization of the corresponding indicators of hard tissues of human teeth is extremely problematic, primarily due to the complexity of conducting experiments and processing their results. For example, the outer layers of enamel have a lower crack resistance index 0,67±0,12 MPa·$\sqrt{м}$, and the inner layers show an increase in crack resistance from 1,13 to 3. The results of data processing from literature sources [10, 11] are given in Table 1.

Table 1

Mechanical properties of hard dental tissues and dental materials

Indicator	Dentin	Enamel	Vittra APS	Z 350 XT	Tetric N-Ceram	Estelite Quick	Charisma Diamond
Modulus of elasticity [GPa]	3,67	5,49	9,50	10,10	7,05	5,95	9,90
Strength [MPa]	538	253	232	120	245	230	115
Fracture toughness [MPa$\sqrt{м}$]	6,00	0,67	1,18	1,19	0,84	0,83	1,30
Hardness	68	343	95	76	58	70	70

Further calculations are more convenient if Eq. (2) is written in the form:

$$I_{qe} = \frac{4}{\left(\frac{E^t}{E^m} + \frac{\sigma^t_{\max}}{\sigma^m_{\max}} + \frac{K^t_c}{K^m_c} + \frac{HK^t}{HK^m} \right)}, \quad (4)$$

where I_{qe} is a complex indicator of the material quality according to the selected characteristics, which is determined separately for the enamel and dentin of the tooth.

Calculations according to the developed methodology for the selected materials are given in Table 2.

Table 2

Complex quality index of composite restorative materials

Indicator	Dentin	Enamel	Vittra APS	Z 350 XT	Tetric N-Ceram	Estelite Quick	Charisma Diamond
I_{qe} relative to enamel	1,00	1,00	0,68	0,52	0,47	0,52	0,49
I_{qe} relative to dentin	1,00	1,00	0,47	0,37	0,36	0,36	0,38

The quality assessment of the above composite materials can, of course, be carried out by comparing their individual mechanical properties or by their relation to the corresponding characteristics of enamel and dentin. Let us present some results of this analysis.

From Table 1 it follows that the highest modulus of elasticity has the Z 350 XT, the highest compressive strength — Tetric N-Ceram, crack resistance – Charisma Diamond, and hardness – Vittra APS. The smallest values of the parameters, listed in the same order, are for Estelite Quick, Charisma Diamond, Estelite Quick and Tetric N-Ceram. The above does not in any way imply a conclusion: which material is better to use in medical practice. If we do not take into account the specific dental aspects of a particular case, and consider, for example, the compressive strength of the material, it is better to use Tetric N-Ceram. At the same time, this material has a relatively low hardness.

Thus, for a rational choice of a restorative composite from a number of available preparations, it is necessary to determine a complex (summary) quality index of materials to the properties of hard tooth tissues. In our case, we are talking about mechanical properties. Depending on the treatment protocol, this may be the characteristics of enamel or dentin.

In this regard, as follows from the calculations given in Table 2, of the photopolymers analyzed above, Vittra APS is the best, the quality coefficient of which is 0,68 relative to enamel, and 0,47 – relative to dentin. Tetric N-Ceram and Charisma Diamond turned out to be problematic relative to enamel with indicators of 0,47 and 0,49, respectively; Z 350 XT, Tetric and Estelite Quick occupy the middle step with a coefficient of 0,52.

As for the comparison with dentin, Vittra APS is again the best, and all other materials, inferior to it in terms of the combined indicator, have almost the same coefficient – from 0,36 for Tetric N-Ceram to 0,38 for Charisma Diamond.

As expected, for all the considered materials the quality coefficient I_{qe} turned out to be less than one, although, theoretically, it can exceed it due to some parameter of the composite being much larger compared to enamel or dentin. At the same time, it is doubtful that an artificial dental material can surpass a natural one in all indicators.

The combined quality factor for dentin for all materials is noticeably lower compared to the indicator for enamel. This implies that the considered photopolymers, if possible, are better used when eliminating enamel defects. In general, it can be stated that all the analyzed materials are of high quality. At the same time, by improving one or another characteristic, the overall quality of the materials can be improved. Let us follow the example of calculating the combined quality factor by changing one of the four mechanical quantities. At the same time, we will leave the other three included in Eq. (4) unchanged. Strictly speaking, all the characteristics are interconnected, but for an evaluative analysis of the influence of individual indicators on the materials quality, it is advisable to consider these dependencies. The results of calculating the combined materials quality factor in relation to enamel are presented in Fig. 1–4. The numbering of the curves further corresponds to the materials: 1 – Vittra APS, 2 – Z 350 XT, 3 – Tetric N-Ceram, 4 – Estelite Quick, 5 – Charisma Diamond.

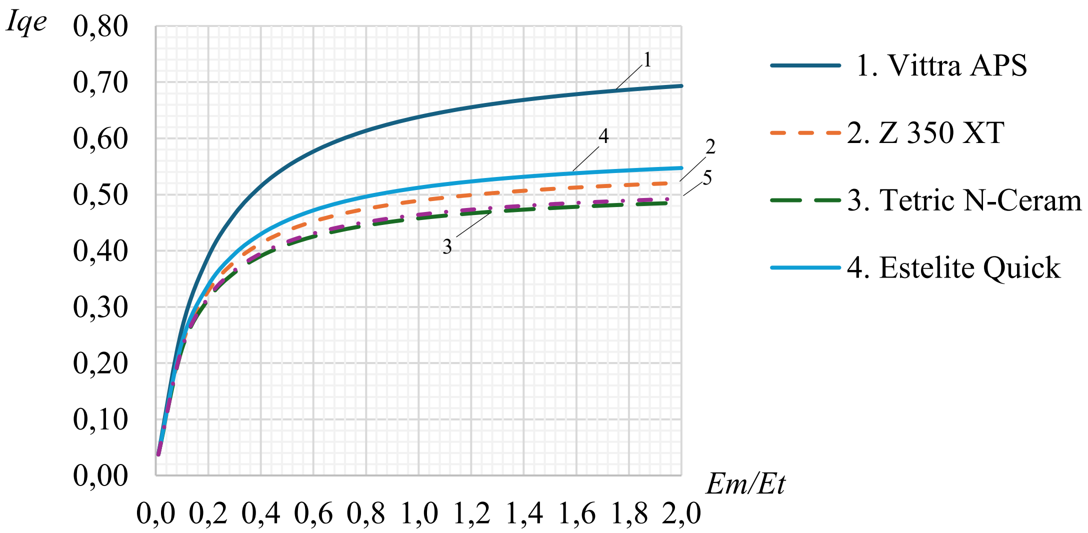

Fig. 1. Dependence of the materials quality factor on the relative elasticity modulus

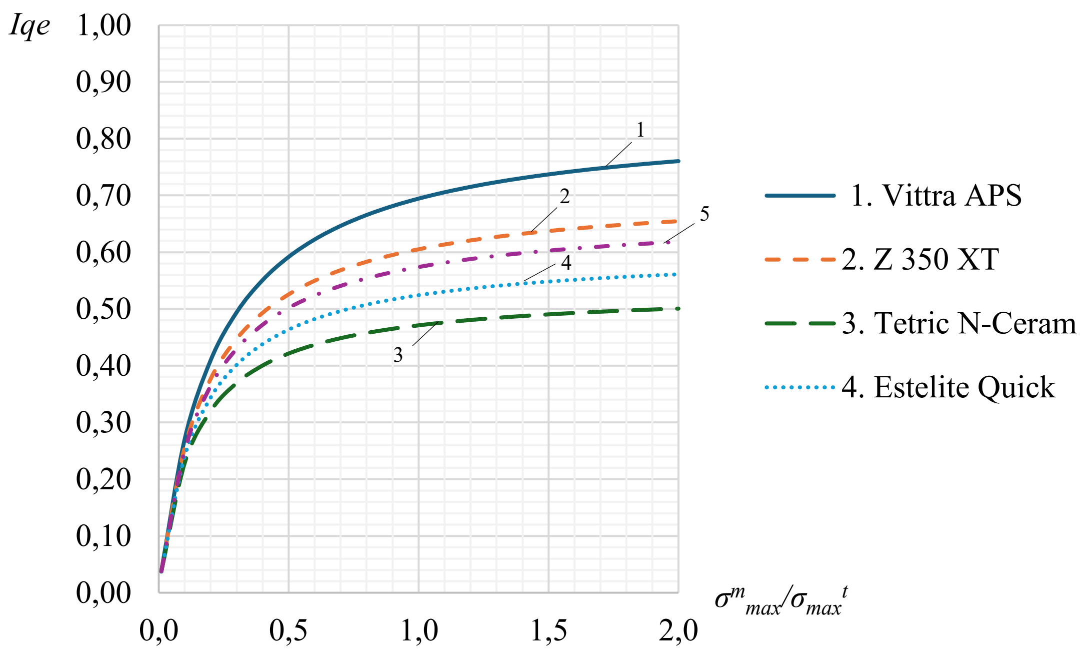

Fig. 2. Dependence of the quality factor on the relative compressive strength

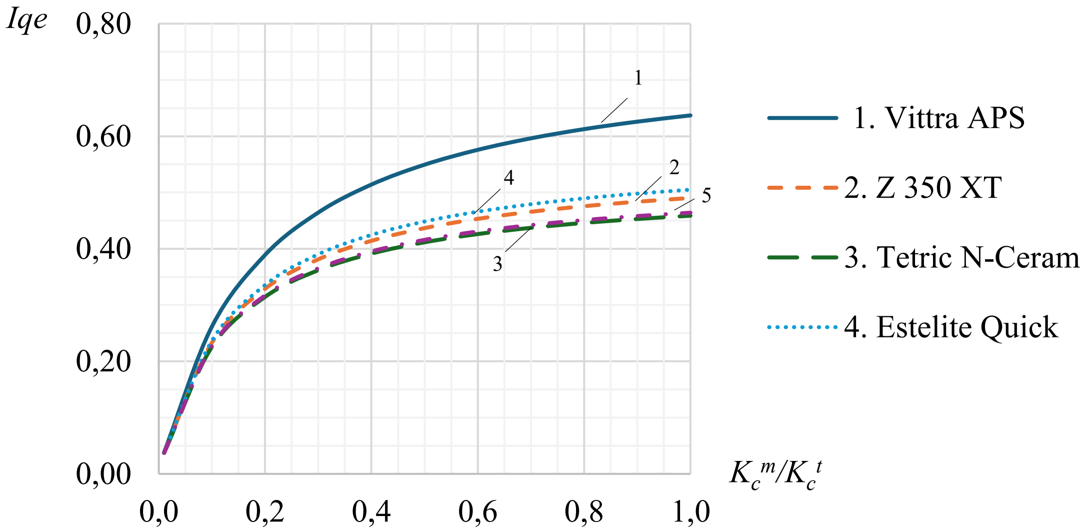

Fig. 3. Dependence of the quality factor on the relative fracture toughness

Similar dependencies can be obtained by calculations in relation to dentin.

Four mechanical characteristics were chosen as the basic parameters. In the future, regarding the materials qualimetric assessment using the concept of «harmonic mean», there are no fundamental restrictions on increasing the number of basic characteristics. This may be an indicator of biocompatibility, an economic component, etc.

A comparative analysis of the results obtained in relation to tooth enamel confirms the conclusion that it is impossible to generally assess the quality of the studied materials by any one mechanical characteristic. Thus, if we take the numbering of materials adopted in Fig. 1-4, then the distribution of places by the best modulus of elasticity will look as follows: 2 – 5 – 1 – 3 – 4; higher strength: 3 – 1 – 4 – 2 – 5; better fracture toughness (crack resistance): 5 – 2 – 1 – 3 – 4; greater hardness: 1 – 2 – 4,5 – 3.

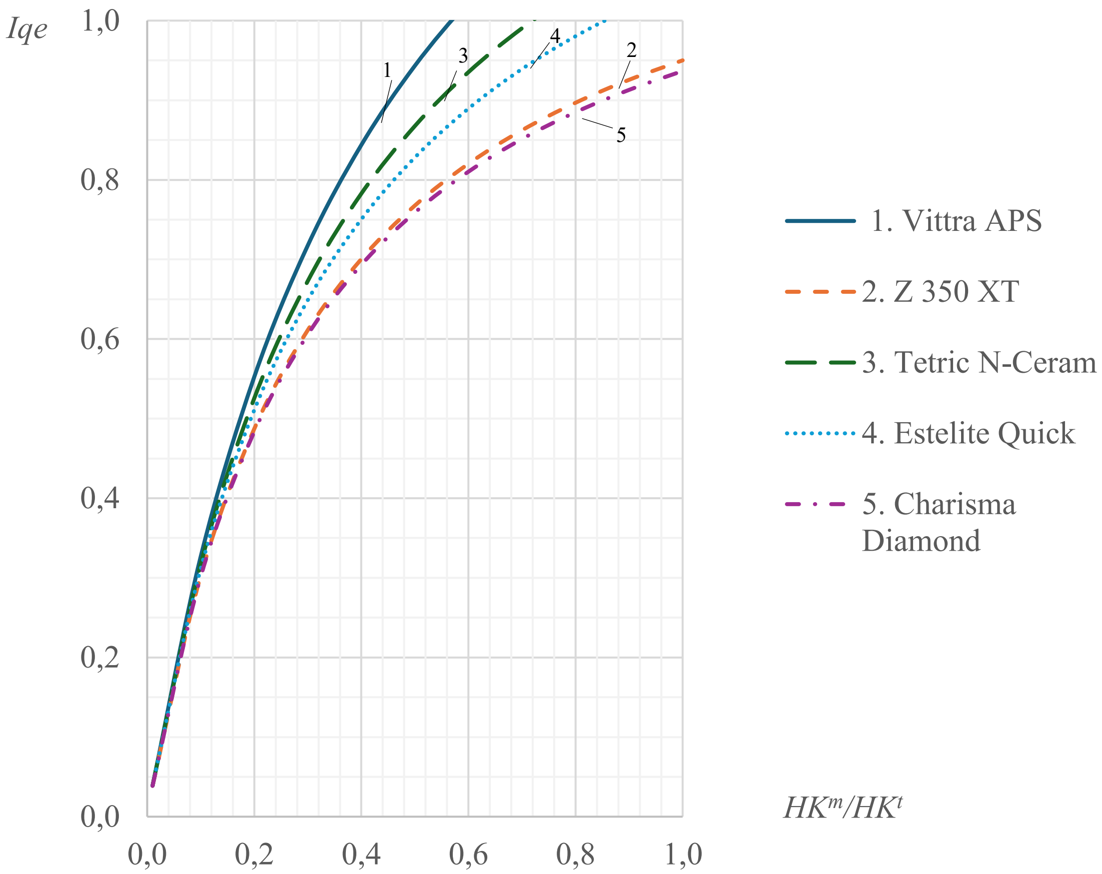

Fig. 4. Dependence of the quality factor on the relative hardness

At the same time, the quality assessment of the same materials by the combined quality indicator, with the same ratios to enamel of the modulus of elasticity, strength, crack resistance and hardness, the distribution becomes completely different: 1 – 4 – 2 – 5 – 3; 1 – 2 – 5 – 4 – 3; 1 – 4 – 2 – 5 – 3; 1 – 3 – 4 – 2 – 5.

It is quite clear that with a number increase in the basic characteristics in the adopted approach, the quality indicator of the material can change significantly.

The presented comparative analysis does not contradict the conclusion obtained above – the highest quality indicator in terms of mechanical properties has the Vittra APS material, determined by the available properties (see table 1). It also follows from Fig. 1–4 that a relatively small change in the value of the mechanical characteristic (programmed or determined incorrectly) can lead to a significant change in the combined quality indicator. This is particularly evident when varying the ratio of the hardness of the restorative composite to the hardness of the enamel (see fig. 4). For example, for the Vittra APS photopolymer, changing the ratio $\frac{HK^m}{HK^t}$ from 0,2 to 0,3, with other material characteristics held constant, increases the calculated quality factor from 0,55 to 0,74. For other mechanical properties, this is less evident.

Conclusions. Due to the large number of restorative dental materials, a method for their qualimetric assessment is extremely necessary.

Analysis of individual materials mechanical properties does not give a complete picture for their quality and can lead to erroneous conclusions.

For the restorative nanohybrid photopolymers quality assessment, a method based on the harmonic mean concept of the artificial materials elasticity modulus, strength, crack resistance and hardness to the corresponding characteristics of natural enamel and dentin has been proposed.

Systematization and processing of the dental materials mechanical properties allowed calculations of the proposed complex indicator for their quality, reduced to the dental enamel and dentin properties. Due to the significant difference in the structure and enamel and dentin properties, it is advisable to determine the material quality indicator separately.

For qualimetric assessment of materials using the considered method, there are no fundamental restrictions on basic parameters increasing number.

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АНОТАЦІЯ

Мета. Аналіз механічних характеристик стоматологічних матеріалів у порівнянні з властивостями емалі та дентину зубів та розробка методу кваліметричної оцінки ефективності використання сучасних біомеханічних реставраційних матеріалів у малоінвазивній стоматологічній практиці.

Методика. Для кількісної оцінки реставраційних матеріалів запропоновано та обґрунтовано метод, заснований на концепції середнього гармонійного співвідношення модуля пружності, міцності, тріщиностійкості та твердості штучних матеріалів до відповідних властивостей природної емалі та дентину. Показники якості емалі та дентину прийняті такими, що дорівнюють одиниці. Відповідно, що чим ближче показник якості реставраційного матеріалу до одинці, тим він ближче до характеристик природнього матеріалу за обраним критерієм, тобто є кращим з варіантів, що розглядаються.

Результати. Систематизовано механічні параметри п'яти реставраційних композитних матеріалів та проведено розрахунки запропонованого комплексного показника їх якості, зведеного до властивостей емалі та дентину зубів. Порівняльний аналіз отриманих результатів по відношенню до зубної емалі підтверджує висновок про неможливість загальної оцінки якості досліджених матеріалів за якоюсь однією механічною характеристикою. Проведені розрахунки підтверджують можливість застосування запропонованої методики.

Наукова новизна. Встановлені залежності між базовими параметрами, прийнятими для оцінки механічних властивостей стоматологічних нанокомпозиційних матеріалів (модулем пружності, міцністю, тріщиностійкістю, твердістю), можуть бути використані для вдосконалення методів кваліметричної оцінки біомеханічних матеріалів. Для кваліметричної оцінки матеріалів за розглянутою методикою немає принципових обмежень до збільшення кількості базових параметрів.

Практична значимість. Отримані результати досліджень реставраційних композитних матеріалів за комплексним показником якості можуть сприяти достовірній практичній оцінці існуючих та нових стоматологічних матеріалів для зниження ризиків та підвищення ефективності їх практичного використання.

Ключові слова: *малоінвазійна стоматологія, нанокомпозит, біосумісність, кваліметрична оцінка, фотополімер, властивості матеріалів.*

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