POISSON'S RATIO OF DENTIN AND ENAMEL AS ANISOTROPIC MEDIA WITH HEXAGONAL SYMMETRY

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Abstract. In this paper, the orientation dependence of the Poisson's ratio of teeth's dentin and enamel on the basis of matrices of elastic constants and the compliance coefficients of hexagonal crystals, such as crystals of dentine hydroxyapatite, was obtained for the first time. The results of calculating the Poisson's ratios of dentin and enamel as a crystalline system with a hexagonal structure are presented in the form of tables and diagrams in the polar and Cartesian coordinate systems. It is shown that the maximum value of the Poisson's ratio of dentin (0.54) is greater than the upper limit for the Poisson's ratio of isotropic materials, including known restoration materials, which in some cases may reduce the quality of restorations. The effective elastic characteristics of dentine and enamel, including Poisson's ratio using different averaging methods, are calculated.
Key words: *enamel, dentin, Poisson's ratio, crystals of hydroxyapatite.*

INTRODUCTION

Elastic properties of hard tissues of tooth and hydroxyapatite, as their mineral component, quite often cause interest among researchers [1-8]. However, a number of aspects of this subject, in particular the value of the Poisson's ratio (coefficient of transverse deformation) of dentine and enamel as anisotropic media with hexagonal symmetry, remain relevant to the end. The study was conducted on the basis of two different methods of calculation [9, 10].

According to modern concepts, the range of possible values of the Poisson's ratio [11, 12] can be negative $\mu<0$ (auxetics), and more than 0.5. For dentin and enamel the "technical" coefficient according to the literature data lies in the range of 0.29-0.33 [13], for example, according to the results of ultrasonic measurements for dentin, it is equal to 0.32, in enamel – 0.28 [8].

THE STUDY OF ANISOTROPY POISSON RATIO OF DENTIN AND ENAMEL

It is believed that dentin is a biocomposite and consists of approximately 45-70 % of inorganic material [7, 14] in the form of hydroxyapatite crystals. Crystals of hydroxyapatite are located between the collagen fibers and the class of symmetry belong to hexagonal crystal structure. The mineral base of enamel is represented by hexagonal crystals of hydroxide, carbonate, chlorine, fluorapatite, and enamel prisms are the main structural formation. Therefore, there is every reason to consider dentine and enamel as anisotropic media, which means that their elastic properties are described by the matrix of elastic constants c_{ij} or compliance coefficients s_{ij} .

The Poisson ratios of such a medium in the general form can be defined as

$$\mu_{kl} = -\frac{\varepsilon_{ll}}{\varepsilon_{kk}}, \tag{1}$$

where ε_{kl} – components of the strain tensor. As a result, hexagonal systems, dentin and enamel are also described by two Poisson's ratios μ'_{31} and μ'_{32} [10]. According to the literature data, the values of the elastic constants of dentin and enamel are well known [5, 6], so knowing them, we can calculate the coefficients of compliance and the Poisson's ratio of dentin and enamel by the corresponding formulas [10, 15] for hexagonal crystals.

$$c_{11} + c_{12} = \frac{s_{33}}{s}, \quad c_{11} - c_{12} = \frac{1}{s_{11} - s_{12}}, \quad c_{13} = -\frac{s_{13}}{s}$$
$$c_{33} = \frac{s_{11} + s_{12}}{s}, \quad c_{44} = \frac{1}{s_{44}}, \quad c_{66} = \frac{1}{s_{66}}, \quad s = s_{33}(s_{11} + s_{12}) - 2s_{13}^2 , \tag{2}$$

$$\mu'_{31} = -[\sin^2\psi \sin^2\theta \cos^2\theta (s_{11} + s_{33} - s_{44}) + (\cos^2\theta - \sin^2\theta \cos 2\theta \sin^2\psi) s_{13} + \sin^2\theta \cos^2\psi s_{12}] / s'_{33} \tag{3}$$

and

$$\mu'_{32} = -[\cos^2\psi \sin^2\theta \cos^2\theta (s_{11} + s_{33} - s_{44}) + (\cos^2\theta - \sin^2\theta \cos 2\theta \cos^2\psi) s_{13} + \sin^2\theta \sin^2\psi s_{12}] / s'_{33}, \tag{4}$$

where

$$s'_{33} = \cos^4\theta s_{33} + \sin^2\theta \cos^2\theta (2s_{13} + s_{44}) + \sin^4\theta s_{11} , \tag{5}$$

Table 1. Elastic constants of dentin and enamel (GPa)

Material	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}
Dentin	37.00	16.60	8.70	39.00	5.70
Enamel	115.00	42.40	30.00	125.00	22.80

Table 2. Compliance coefficients of dentin and enamel (GPa^{-1})

Material	s_{11}	s_{12}	s_{13}	s_{33}	s_{44}
Dentin	0.0346	-0.0145	-0.0045	0.0276	0.1754
Enamel	0.0104	-0.0034	-0.0017	0.0088	0.0439

θ и ψ – Eulerian angles (describing the rotation of an absolutely rigid body in a three-dimensional Euclidean space). Orthogonal system x_i has the Ox_3 axis parallel to the <c>-axis of the crystal.

Equation (4) gives Poisson's ratio for an extension along $Ox_3^{'}$ and a contraction along $Ox_2^{'}$, equation (3) gives Poisson's ratio for a contraction in the perpendicular direction $Ox_1^{'}$.

For an isotropic solid $s_{11} = s_{22} = s_{33}$, $s_{44} = s_{55} = s_{66} = 2(s_{11} - s_{12})$, $s_{12} = s_{13} = s_{23}$ and equation (3), (4) and (5) are reduced to $s_{33}^{'} = s_{11}$, $\mu_{32}^{'} = \mu_{31}^{'} = -s_{12} / s_{11}$, so that Poisson's ratio is independent of orientation, what we wanted to prove.

Values of elastic constants c_{ij} and compliance coefficients s_{ij} of dentin and enamel are presented in Table 1 and 2.

The results of calculating the Poisson coefficients (directional dependence) of the dentin and enamel as crystal systems with a hexagonal structure are shown in Figure 1 and Figure 2.

Worthy of attention approach based on calculation of extreme values of the Poisson ratio of crystalline media and create isosurfaces of the coefficient in space [9, 16]. The results of calculating the coefficients of the dentin and enamel Poisson as a crystal hexagonal structure are presented in Table 3 and Figure 3.

All graphics (Figure 1-3) clearly show the pronounced anisotropic behavior of the Poisson's ratio of dentin and enamel crystals. Its values, depending on the direction in space, vary within a very wide range (4.15 times in dentin and 2.94 times in enamel). This number of times can be called the anisotropy coefficient for the Poisson ratio.

Note the anomaly high value of the maximum value of the Poisson's ratio (0.534-0.54) along a number of directions, which is extremely unusual for materials. This means that the compression of the local areas of the dentin along these directions will increase their volume, and when stretched – on the contrary, decrease. The elastic behavior under load of the restoration material is fundamentally different (Poisson's ratio of the filling material is significantly less than 0.5, for example, according to [17] it is between the values of 0.24 to 0.35 for dental composite materials), so its volume decreases when compressed and increases when stretched. This discrepancy in the deformation behavior at the boundary of heterogeneous media of the filling material and dentin can lead to the formation of overstress domains at this boundary, to the weakening of adhesion of the restoration material with dentin and, as a negative result, the degradation of fixation and the often encountered situation of destruction of direct and sometimes indirect restoration, especially composite materials.

1. The average of the Poisson's ratio of dentine and enamel.

The average value of the Poisson's ratio of dentine and enamel can be obtained by applying the formulas (3-5) and the expression [10]:

$$< \mu_{ij}^{'} >= \frac{1}{2\pi} \int_0^{\pi} \int_0^{\pi} \mu_{ij}^{'}(\theta, \psi) \sin\theta d\theta d\psi . \tag{6}$$

Numerical calculations of this integral in Mathcad software give the results: 0.312 for dentine and 0.286 for enamel, which is very well consistent with the data of ultrasonic measurements [8].

Table. 3. Extreme values of Poisson's ratio (μ_{min}, μ_{max}) for dentine and enamel, values of Poisson's ratio in particular orientations and "anisotropy coefficient" μ_{max} / μ_{min}

Material	μ_{max}	μ_{min}	$\mu_{[2\bar{1}\bar{1}0],[0001]}$	$\mu_{[01\bar{1}0],[2\bar{1}\bar{1}0]}$	$\mu_{[0001],[2\bar{1}\bar{1}0]}$	μ_{max} / μ_{min}
Dentin	0.54	0.13	0.16	0.13	0.42	4.15
Enamel	0.47	0.16	0.19	0.16	0.33	2.94

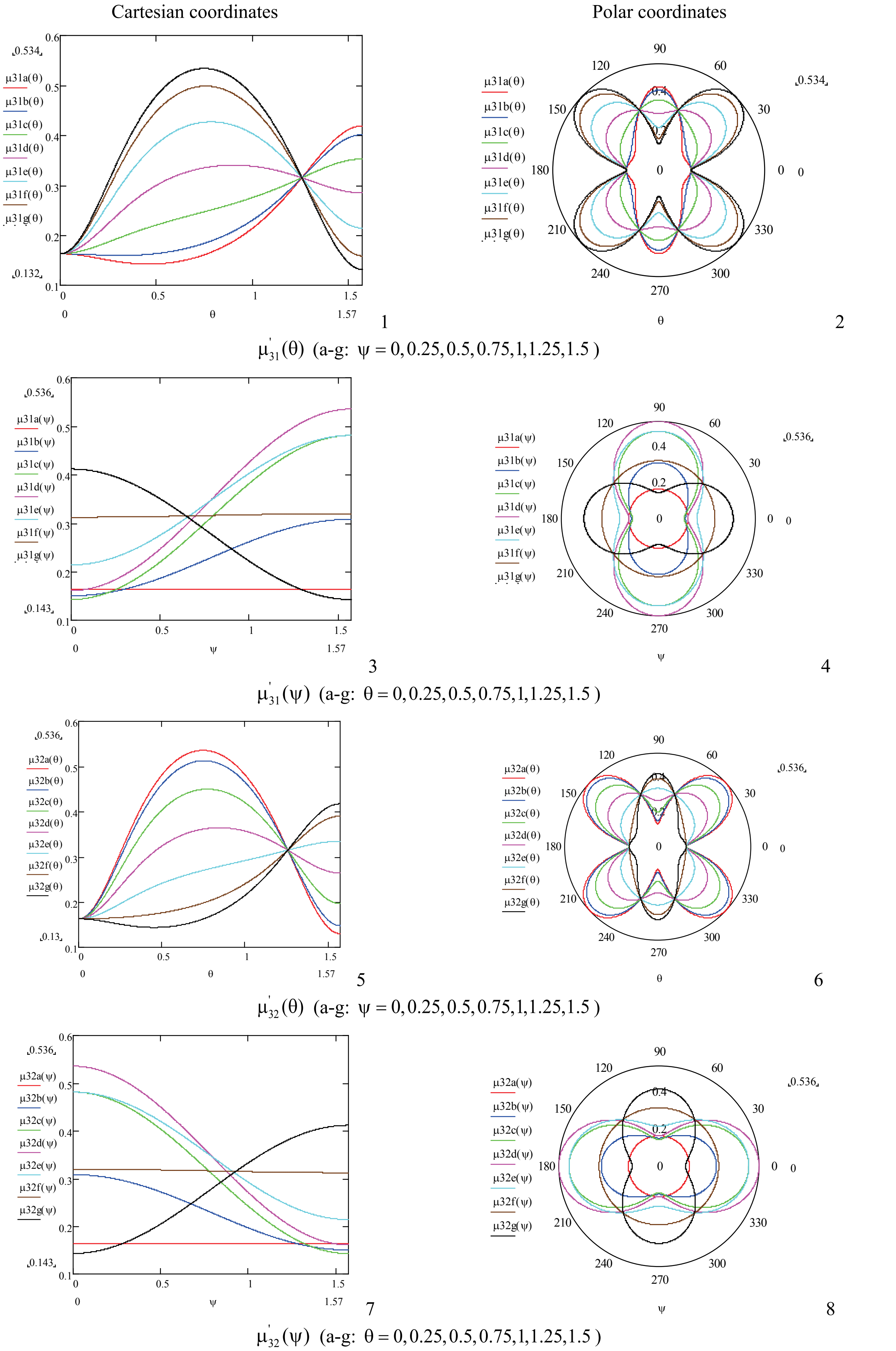
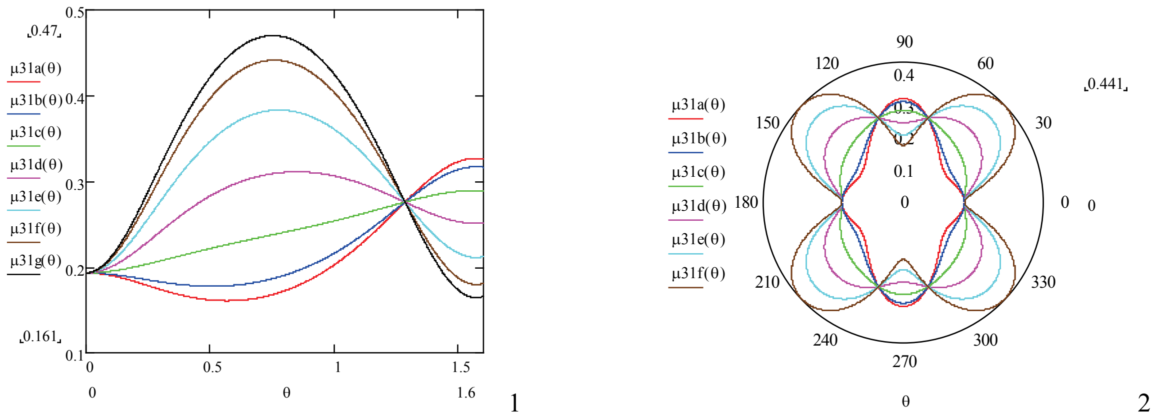
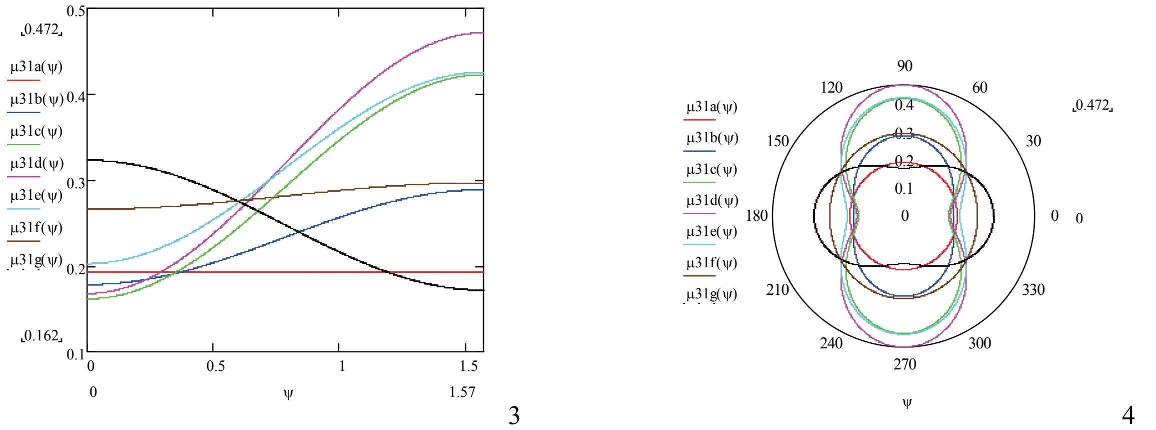


Figure 1. The Poisson's ratio μ'_{31} (1-4) and μ'_{32} (5-8) of dentin for different directions θ and ψ

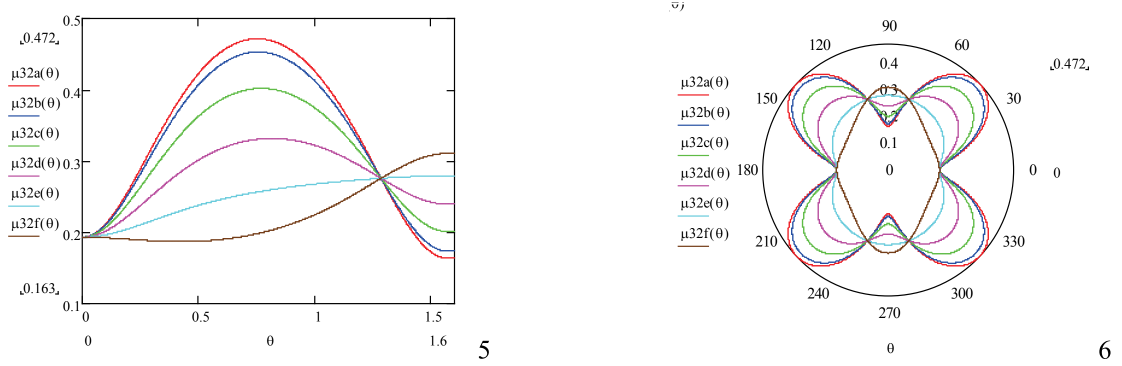
Cartesian coordinates Polar coordinates



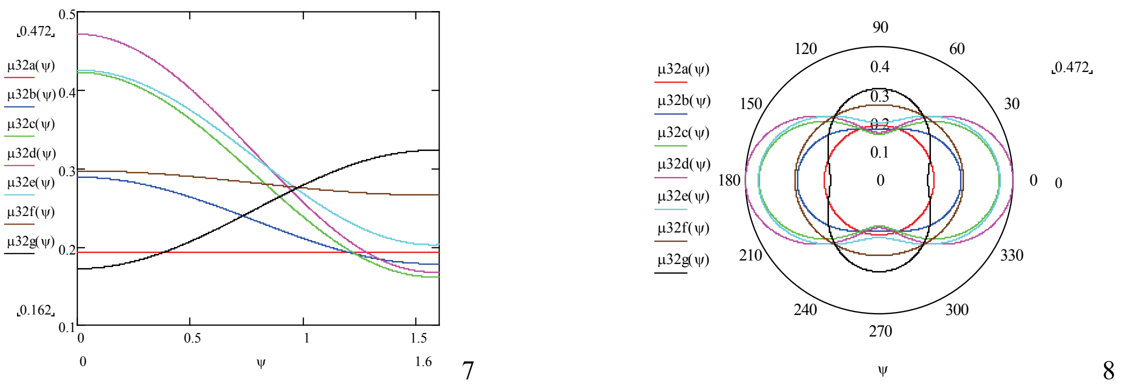
$\mu'_{31}(\theta)$ (a-g: $\psi = 0, 0.25, 0.5, 0.75, 1, 1.25, 1.5$)



$\mu'_{31}(\psi)$ (a-g: $\theta = 0, 0.25, 0.5, 0.75, 1, 1.25, 1.5$)



$\mu'_{32}(\theta)$ (a-g: $\psi = 0, 0.25, 0.5, 0.75, 1, 1.25, 1.5$)



$\mu'_{32}(\psi)$ (a-g: $\theta = 0, 0.25, 0.5, 0.75, 1, 1.25, 1.5$)

Figure 2. The Poisson's ratio μ'_{31} (1-4) and μ'_{32} (5-8) of enamel for different directions θ and ψ

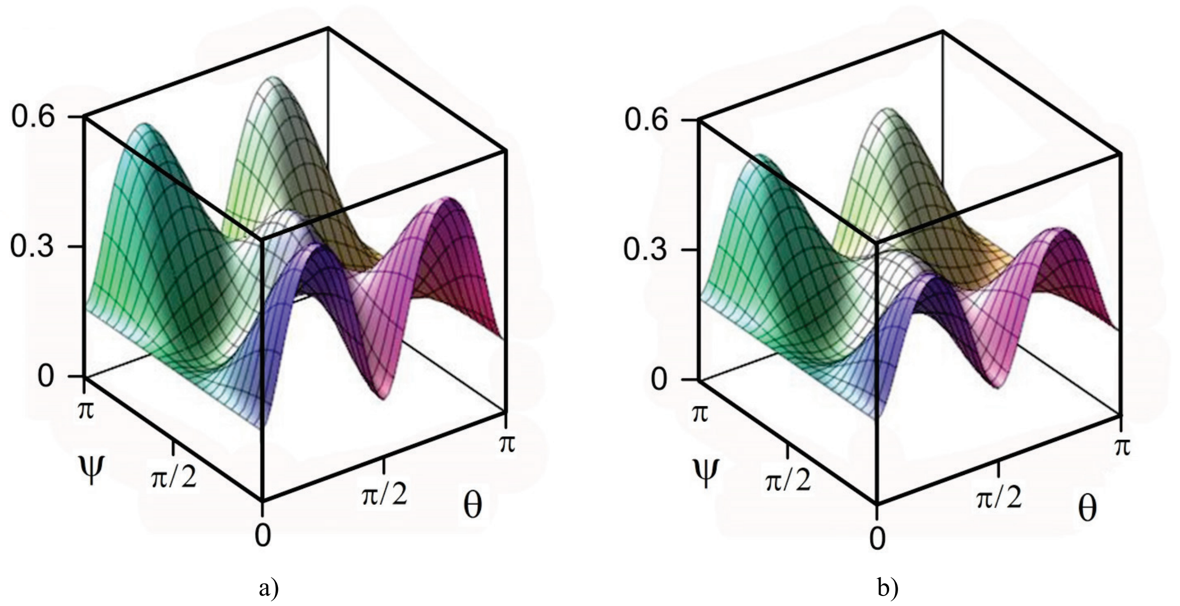


Figure 3. Variability of the Poisson's ratio of dentin (a) and enamel (b) in space

2. Calculation of the effective value of the Poisson's ratio of dentine and enamel on the basis of their elastic constants and compliance coefficients.

On the basis of data obtained on single crystals we can predict the elastic properties of dentin and enamel as microinhomogeneous materials [18].

According to the Voigt averaging, the module of all-round compression and the shear modulus for hexagonal crystals are equal respectively

$$K_V = \frac{2c_{11} + c_{33} + 2(c_{12} + 2c_{13})}{9}$$
$$G_V = \frac{7c_{11} + 2c_{33} - 5c_{12} - 4c_{13} + 12c_{44}}{30}. \quad (7)$$

In the approach proposed by Reuss, the averaging of the compliance tensors is performed, as a result of which for the hexagonal lattice we obtain

$$\frac{1}{K_R} = 2s_{11} + s_{33} + 2(s_{12} + 2s_{13})$$
$$\frac{1}{G_R} = \frac{2(7s_{11} + 2s_{33} + 3s_{44} - 5s_{12} - 42s_{13}}{15}. \quad (8)$$

In many cases, a good agreement with the experimental data gives the proposed by Hill arithmetic mean value, found by the averaging for Voigt and Reuss, namely

$$K_H = \frac{1}{2}(K_V + K_R),\ G_H = \frac{1}{2}(G_V + G_R). \quad (9)$$

Keeping in mind that two modules are independent in the isotropic approximation, we can write expressions for E_H and μ_H as functions K_H and G_H:

$$\langle E_H \rangle = \frac{9K_H G_H}{3K_H + G_H},\ <\mu_H> = \frac{3K_H - 2G_H}{6K_H + 2G_H}. \quad (10)$$

Table 4 shows the values of the averaged elastic modules and the Poisson's ratio of dentine and enamel, calculated from the values of elastic constants and compliance coefficients using the described averaging methods used for single-phase hexagonal polycrystals.

Table 4. Averaged elastic modules and Poisson's ratio of dentine and enamel

Material	K_V	G_V	K_R	G_R	K_H	G_H	E_H	μ_H
Dentin	20.11	9.59	20.03	8.21	20.07	8.90	23.26	0.31
Enamel	62.20	33.22	62.20	30.54	62.20	31.88	81.69	0.28

Note that the calculated values of μ_H are in good agreement with the known experimental data [8] and results of section 3 for $<\mu'_{ij}>$.

SUMMARY

1. Dentin and tooth enamel are not isotropic media due to the symmetry of their mineral component – hydroxyapatite crystals.

2. The expressed anisotropy of the Poisson's ratio of dentine and enamel is established on the basis of calculations by formulas of elastic constants and compliance coefficients for hexagonal symmetry. The maximum value of the Poisson's ratio of dentine (0.534-0.54) is more than 4 times (4.15) higher than the minimum (0.13).

3. The maximum value of the Poisson's ratio of dentine is higher than the upper limit for the Poisson's ratio of isotropic, including restoration materials used in dentistry, which can locally affect the quality of restorations. In this context, it is suggested that the established elastic anisotropy of the dentin model with crystal hexagonal symmetry is a clinically undesirable factor.

4. A more careful analysis of the elastic anisotropy of the hard tissues of the tooth as a mineral-organic complex and a microinhomogeneous heterophase system is possible with the involvement of the theory of anisotropic media with a crystallographic texture (despite the fact that all the prisms of minerals in the dentine and enamel have the same or similar crystal structure, they differ in the mutual orientation of the crystallographic axes). Further analysis is based on the knowledge of the spatial distribution of the crystallographic axes of individual mineral prisms.

5. The study of the anisotropy of dentine and enamel as an anisotropic inhomogeneous medium is of practical importance in the study of the strength of tooth tissues and the quality of restorations.

6. The values of the Poisson's ratio of enamel are not fundamentally different from those of dentin. They are still quite large and indicate anisotropy of elastic properties of tooth enamel, although to a lesser extent: $\mu_{max} / \mu_{min} = 2.94$.

7. Calculation of effective Poisson's ratios of hard tooth tissues based on elastic constants and compliance coefficients and different averaging methods gives results that are in good agreement with empirical data.

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