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STUDY OF STRUCTURAL AND SPECTRAL CHARACTERISTICS OF CRYSTAL $Y_3Al_5O_{12}$, Al_2O_3 AND $SrTiO_3$ DOPED BY 3d- OR 4f- IONS

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Abstract: The subject of our research is a study of the effects of various treatments on the structural and spectral characteristics of oxides ($Y_3Al_5O_{12}$, Al_2O_3 and $SrTiO_3$) belonging to the group of ionic crystals with a wide energy band gap. We have investigated the dielectric and optical characteristics of single laser crystals of $Y_3Al_5O_{12}$ (YAG) doped by ions from the group of iron (3d-), Al_2O_3 single crystal and $SrTiO_3$ crystals doped by 3d and 4f- ions. Dielectric properties of the investigated single crystals were analyzed using dielectric spectroscopy (80 kHz – 15 MHz) in a wide temperature range (50 – 400 K). The comparison of the temperature dependence of the dielectric permittivity (ε_r) and dielectric loss ($tan\delta$) at different test frequencies for undoped and doped crystals was performed. The optical properties were studied on the basis of the absorption spectra in the UV-Vis region. The experiment results showed that presence of 3d dopants in YAG crystal caused a displacement of the absorption edge and appearance of characteristic peaks. The differences observed in the absorption spectra were probably the result of the 3d ions incorporation on two possible symmetrically different positionings of aluminum ions –tetrahedrical and octahedrical– in the YAG crystal lattice. The dielectric spectroscopy measurements for samples of $SrTiO_3$ doped by 4f ions showed anomalous behaviors of the dielectric permittivity at temperatures around the temperature of the structural phase transition 105 K.

Keywords: $Y_3Al_5O_{12}$, $SrTiO_3$, doping, dielectric spectroscopy, UV-Vis spectroscopy.

1. INTRODUCTION

This paper presents the results of studying the effect of different treatments on the spectral and structural characteristics of the crystal yttrium aluminum garnet $Y_3Al_5O_{12}$ (YAG), aluminum oxide Al_2O_3 and strontium titanate $SrTiO_3$ (STO).

Due to its good physical and chemical properties, such as chemical and mechanical stability, low thermal conductivity, little thermal expansion due to good optical properties, YAG crystal has a prominent place in technology and medical applications. As a single-crystal, it is used in magnetic memory devices in magneto-optics and microwave engineering. YAG crystal is the host for near-infrared lasers. Since the discovery of Cr^{4+}:YAG, this crystal has gained importance to the technological possibilities of its application in the areas of optical fibers and remote guiding systems [1].

Al_2O_3 has a wide range of applications in technology as well as in high-temperature-material devices for magnetic recordings and laser emitter. Due to the mechanical strength and good electrical insulation, it belongs to the materials of high technological importance [2].

$SrTiO_3$ is an example of ionic crystals of perovskite structure. It is one of the first materials in which the observed uncharacteristic fero-electric behavior occurred. Taking into account the high value of dielectric permeability, which, with lowering of the temperature below 50 K, increases to the value of the order of 10^4, and a small microwave losses, it has become a very attractive material for many high-frequency and microwave applications, especially at low temperatures. It also shows remarkable properties including quantum para-electric behavior, structural phase transitions and superconductivity. Furthermore, the STO is used as a substrate for high-temperature superconducting films. As a result, there is a growing need to determine its static dielectric permittivity with very high accuracy which would allow the processes to be modeled in the widest possible temperature and frequency range [3, 4].

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Doping is a process often used to change the dielectric properties of the material. Small amounts of dopants can change the properties of these intriguing systems. The replacement of cations with ions of different valence or different radii or increasing the concentration of oxygen voids may generate many physical properties such as semi-conductivity, the transition to a conducting state with a low density of charge carriers and even superconductivity at low temperatures [5].

We analyzed the effect of doping 3d ions (Ti, Cr, Fe) on the dielectric and optical properties of YAG mono-crystals, the impact of doping of 3d ions (V, Mn, Fe, Ni) and 4f - (Nd, Sm, Er) on the dielectric and optical properties of mono-crystals of the STO, and the dielectric properties of mono-crystal Al_2O_3.

In this study, the following techniques were used:

- Dielectric spectroscopy in the temperature range 50 – 400 K and in the frequency range 80 kHz –15 MHz.
- UV - Vis optical spectroscopy in the range from 190 to 900 nm at room temperature.

2. SAMPLES AND EXPERIMENT

The studied samples were mono-crystals $Y_3Al_5O_{12}$ and doped YAG:Ti, YAG:Cr, YAG:Fe crystals, which were obtained from the melt by using Czochralski method. The samples were obtained in collaboration with the Laboratory for Materials of The Institute of Radio Electronics in Kharkov. The concentrations of ions (Ti, Cr, Fe) were in the interval at $10^{-3} – 5 \cdot 10^{-1}$ at%. The thickness of the samples was of about 1 mm and 10 mm in diameter.

STO single crystal samples used in this experiment were grown using Verneuil method. Concentrations of 3d ions (V, Mn, Fe, Ni) were at $5 \cdot 10^{-2}$ at% and concentration 4f- ions or rare earth (RE), Nd, Sm, Er at the $2 \cdot 10^{-3}$ at%. The samples were in the form of pellets l = 0.8 – 1 mm thick and with diameter of about d = 10 mm. The color of STO samples doped by Nd, Sm and Er ions was dark gray compared to a transparent STO.

Measurements of the dielectric permeability ε_r and dielectric loss tangent $\tan\delta$ of studied samples were performed in the frequency region of 80 kHz – 15 MHz using the Agilent Precision LCR Meter 4285 device. The tile-shaped samples were placed between the electrodes of the dielectric cells with AC signal. The applied voltage was 1.5 V. The sample temperature was controlled using CTI-Cryogenics Cryodyne closed system and Lake Shore 340 temperature controllers. The data acquisition was performed in the heating mode, where a heating rate of 2 Kmin^{-1} was set. The measurements were carried out in the research laboratories for Solid State Physics at the University of Belgrade. The details of the experimental setup were described in papers [6, 7].

The optical spectra were recorded using a Shimadzu UV– 3600 UV / Vis / Near spectrophotometer in the range of 190 nm to 900 nm. For the purpose of recording the characteristics in the infrared part of the interval in the 4000 – 200 cm^{-1}, the Perkin Elmer 883 spectrometer at room temperature was used [4].

3. RESULTS AND DISCUSSION

3.1. The measurement results and discussion $Y_3Al_5O_{12}$

Yttrium aluminum garnet $Y_3Al_5O_{12}$ is a garnet structure oxide with the formula $A_3B_2'B_3''O_{12}$. Ions A, B_2' and B_3'' are the cations which are located in the positions of different symmetries. Yttrium ions are in the center of dodecahedron, surrounded by 8 oxygen atoms. Aluminum Al ions in the YAG lattice are occupying two positions of different symmetries: $Al_{okt}(B')$ atoms occupy the position with octahedral point group symmetry (C_{3i}), while $Al_{tet}(B'')$ occupy a position with a tetrahedral point group symmetry (S_4). Single elementary cell is large and contains 8 structural formulas, or 160 atoms. This complex structure of yttrium aluminum garnet can be viewed as a network of interconnected octahedron, tetrahedra and dodecahedra whose corners are oxygen atoms, so that each oxygen atom is a member of two dodecahedrons, one octahedron and one tetrahedron [8]. Because of its cubic symmetry, the dielectric characteristics of a YAG crystal are isotropic. According to its dielectric properties, it belongs to the materials with relatively low dielectric losses [9]. The electronic structure of the YAG crystal has been studied less in the theory, and the reason lies in its complex crystal structure.

Dielectric measurements of monocrystalline samples of undoped YAG and doped YAG:Ti, YAG:Cr and YAG: Fe were performed in the frequency range of 80 kHz to 15 MHz at temperatures from 30 to 400 K. Permittivity of $\varepsilon_r(T, f)$ as a function of temperature and the logarithm of frequency for undoped YAG is shown in Figure 1 (a). From the figure it can be seen that the permittivity gradually increased with the increase in the temperature. The trend of temperature dependency remained almost identical for all test frequencies in the studied interval. The dependence of dielectric loss as a function of temperature and frequency for YAG crystal is shown in Figure 1(b). The measured values of dielectric losses were relatively small, of the order of 10^{-4}. The results of $\varepsilon_r(T)$ and $tan\delta(T)$ were in accordance with the published results of other authors at frequencies of 1 kHz, 1 MHz [9, 10]. The Figure 1(b) shows a slight increase in dielectric loss with increasing the temperature. The trend of dependence of $tan\delta(T)$ does not depend almost at all on the test frequencies. The experimental results of the dielectric permittivity and dielectric loss of the doped YAG:Ti and YAG:Cr crystals are shown in Figures 1 (c) - (f).

All these samples showed a temperature dependence of the dielectric permittivity that corresponds to crystals with ionic and covalent bond. For this type of crystal, the permittivity can be described according to M.Lj. Napijalo [11], using the formula:

$$\varepsilon_r(T) = 1 + \frac{C_e}{\theta_e - T}, \tag{1}$$

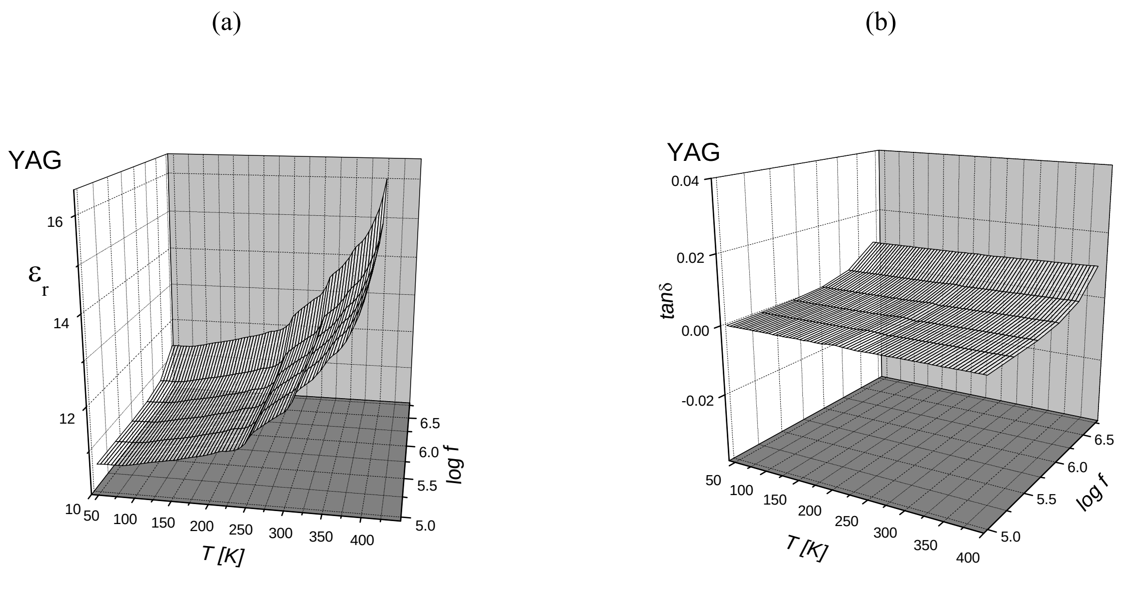
where C_e and θ_e are constants. The existence of this dependence makes it possible to predict the behavior of these materials in a wider temperature range.

A similar dependence trend $\varepsilon_r(T)$ was observed in YAG:Ti, YAG:Cr and YAG:Fe crystals in the temperature range from 50 K to 350 K. However, it can be noticed in Figure 1(c) that at temperatures above 350 K $\varepsilon_r(T)$ they had slight deviations compared to the undoped YAG crystal. This deviation was observed for all doped samples at a temperature higher than 350 K. In the paper [12], the results of dielectric measurements for YAG crystals containing ions Ti, Cr and Fe before and after thermal treatment at a frequency of 1 MHz were published. They were thermally treated by annealing at 600 ° C for 3 h. The results showed that the value of the dielectric permittivity was lower after the annealing, indicating that most likely it was a case of decrease in the concentration of oxygen vacancies. In connection with this, a lowering of the dielectric permittivity in the doped samples can be explained by a decrease in the concentration of oxygen vacancies caused by the increase in the temperature.

All these experimental results demonstrate the important fact that these crystals show a high stability of dielectric characteristics relative to the doping, temperature change and the frequency change.

A mild increase in dielectric permittivity occurring with increasing the temperature was observed for monocrystalline Al_2O_3 sample. Permittivity increased with increasing the temperature. The results for Al_2O_3 dielectric measurements are described and published in [13, 14].

These are important results which describe the dielectric properties of crystals with a large interzonal gap in a wide temperature and frequency range.


(a) (b)

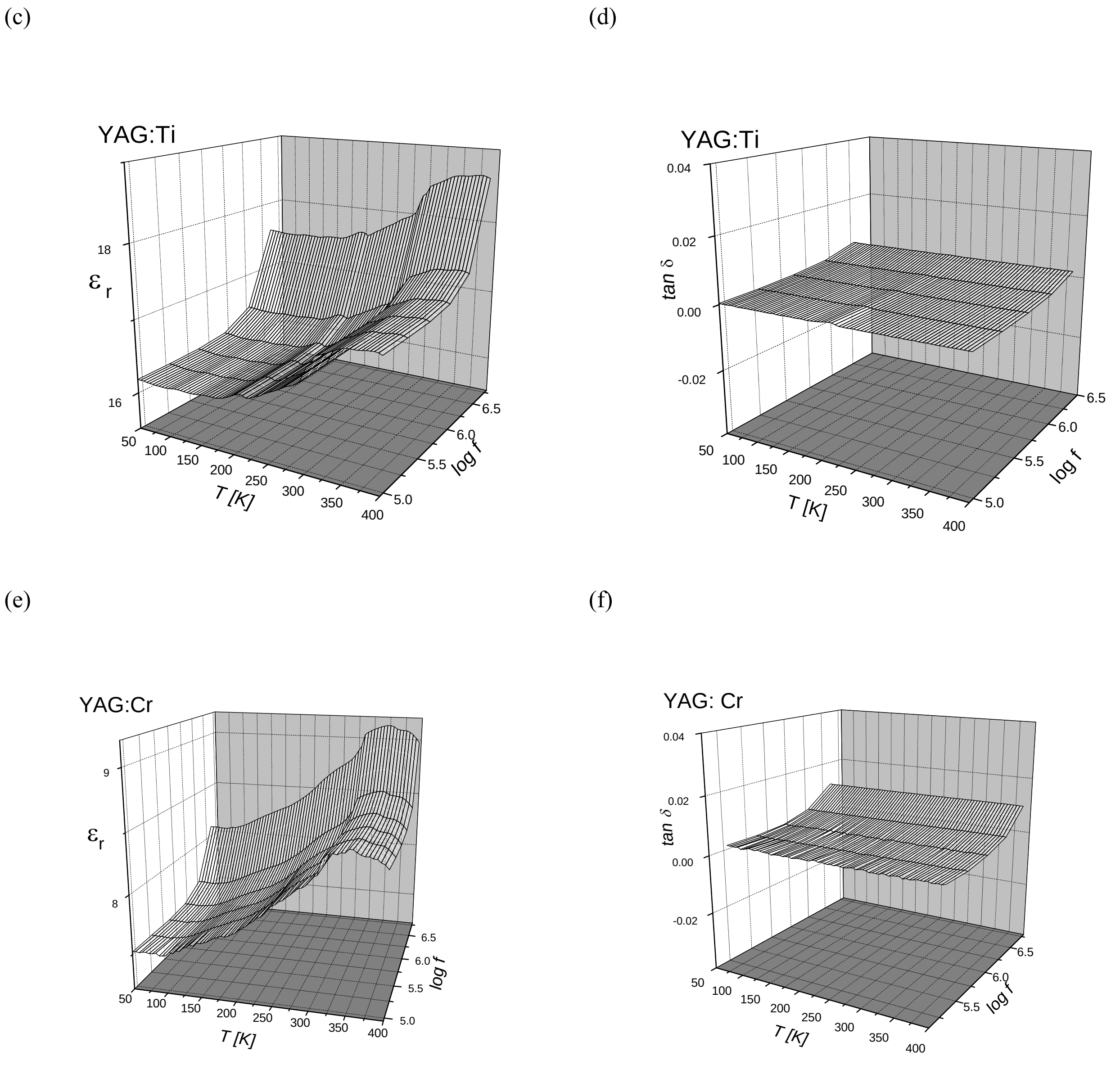


Figure 1. The dielectric permittivity as a function of temperature and the logarithm of the frequency of (a) YAG, (c) the YAG:Ti (e) the YAG:Cr and tan(δ) for (b) YAG, (d) the YAG:Ti, and (f) the YAG:Cr

On the other hand, the optical properties of YAG crystals are very sensitive in relation to the presence of impurities. Based on the preliminary experimental results, it may be said that the optical absorption of YAG crystals in the energetic field of about 4.5 eV to 6.4 eV is greatly influenced by impurity [15]. The absorption of this energy field changes with different dopants in YAG. These differences may stem from differences in crystal growth conditions, the purity of materials and stoichiometry [12]. Also, the absorption in this area changes during the oxidizing and reducing treatments, as well as under the influence of all types of radiation, such as X- and γ- irradiation.

Our study of optical spectra included the recording of transmission spectra of YAG, YAG:Ti, YAG:Cr and YAG:Fe mono-crystal samples in the range of wavelength 190 – 900 nm. Figure 2 (a) shows the transmission spectrum of undoped YAG crystal at room temperature. It was noted that the undoped YAG crystal was transparent at wave lengths greater than 195 nm. On the spectra of doped crystals, Figures 2 (b), (c) and (g), the shift of the absorption edge towards longer wavelengths, i.e. towards lower energies, was observed. The transparency of the samples of YAG:Ti, YAG:Cr and YAG:Fe started at wavelengths of 252 nm, 242 nm, 264 nm respectively. In addition, in the spectra in Figures 2 (b) and (c), it can be observed that additional absorption peaks appeared for the YAG:Ti and YAG:Cr crystals. The observed peaks are shown in Table 1. With regard to the YAG:Ti crystal, the observed absorption peaks had low intensity and were observed at the wavelengths of 390 nm, 480 nm and 560 nm. These absorption peaks corresponded to the abstraction of electrons by oxygen cavities and Ti^{3+} transition in the crystal field. The spectrum of YAG:Cr crystals showed an absorption strip of lower intensity at 330 nm and two very strong absorption bands at about 430 nm and 600 nm. These peaks appeared because Cr^{3+} ions occupied octahedral positions in the YAG crystal grid. Additionally, experimental results, which are based on the theory of valence shifts, indicated that part of the Cr^{3+} ions moved to the valence state Cr^{4+}. Other absorption peaks were not observed for YAG:Fe. Based on the results of luminescent spectra, the Fe^{3+} ions were installed on tetrahedral and octahedral position Al^{3+}.

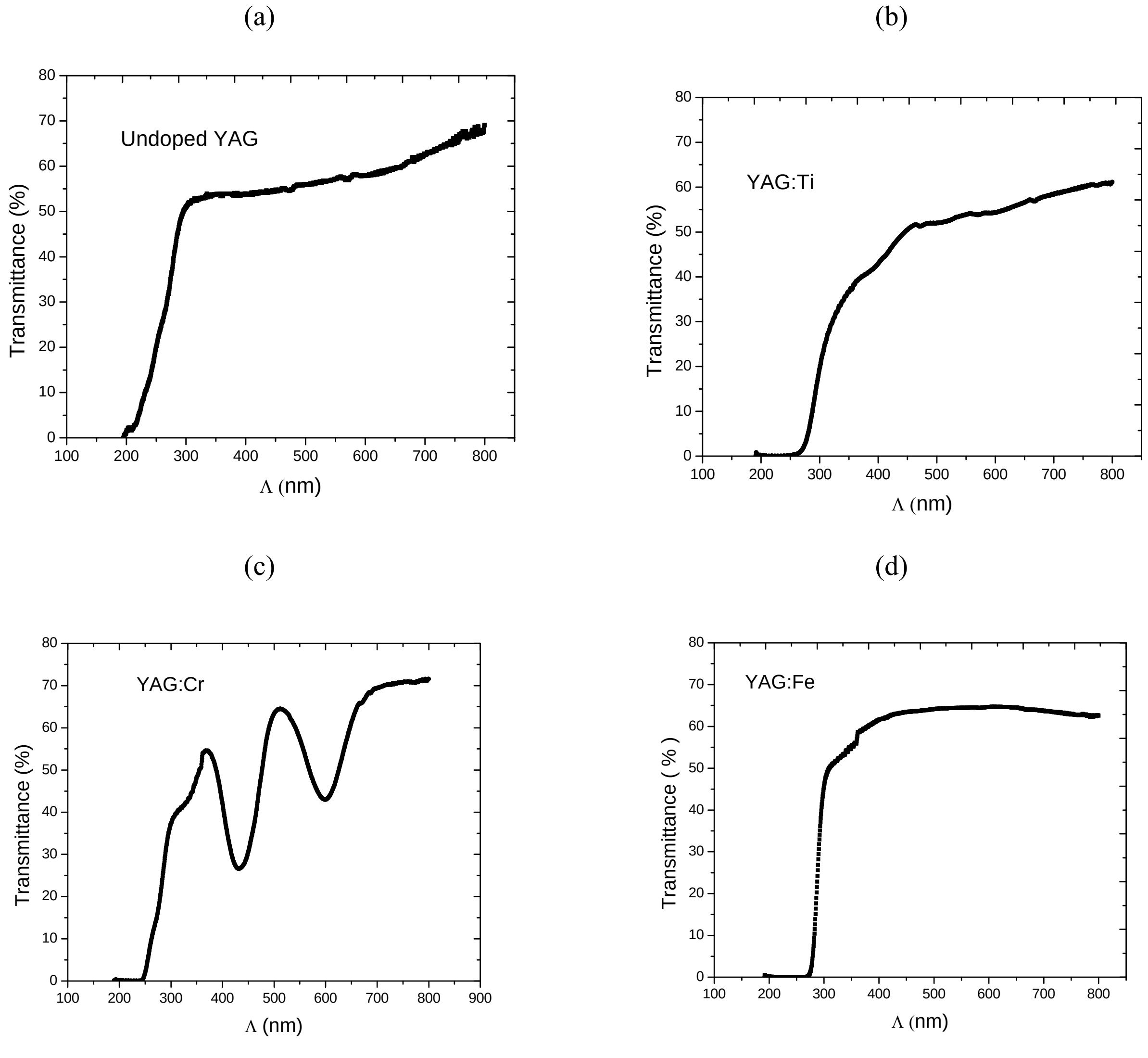


Figure 2. UV-Vis transmission spectra of (a) YAG, (b) the YAG:Ti (c) the YAG:Cr, and (d) the YAG: Fe

The analysis of optical absorption spectra is one of the most important methods for determination of the energy of *Eg* optical gap of the crystal. Based on the spectra $\alpha(h\nu)$, the optical gap is determined by using the relation [16]:

$$(\alpha h\nu) = A(h\nu - E_g)^m \tag{2}$$

where α is absorption coefficient, A – constant not dependent on energy, $h\nu$ – energy, m – exponent which determines the type of electronic transition ($m = 1/2$ for the allowed direct transition, and $m = 2$ for the indirect transition) and *Eg* is an optical energy gap. The optical energy gap for materials YAG and Al_2O_3 belongs to the direct optical transition. The value of the energy gap can be determined by extrapolation method based on $(\alpha h\nu)^2$ dependency of $h\nu$ [7]. Table 1 shows the obtained values of the energy gap for crystals tested at room temperature. The estimated value for the undoped YAG crystal is 6.3 eV. This value is consistent with the experimental data from the study [15]. For the doped YAG:Ti, YAG:Cr and YAG: Fe crystals the obtained values of the energy gap were 4.98 eV, 4.92 eV, 4.53 eV, respectively. These values were significantly lower than the values for the undoped crystals. This is an important result because it tells us about the sensitivity of the optical characteristics of YAG crystals to doping. The maximum deviation was observed for crystals of YAG:Fe.

In addition to measuring optical spectra at room temperature, the optical measurements were carried out at temperatures higher than room temperature (400 K). The results of these measurements showed that the value of the energy gap slowly decreased with the increase of temperature. These changes were very small (only to 0.05 eV), which indicates the optical stability of these materials.

Optical measurements were performed for the oxide Al_2O_3 and showed that the Al_2O_3 crystal was transparent throughout the studied range 190 – 900 nm. Based on the data from the literature, the value of the optical gap is 8.8 eV [17], which is consistent with the transparency in the spectrum.

Table 1. Optical characteristics of samples of monocrystalline YAG, YAG:Ti, YAG:Cr, YAG:Fe

	Start of absorption (nm)	The optical gap, *E*g (eV)	Peaks (nm)
YAG	195	6.31	/
YAG:Ti	252	4.98	390,480,560
YAG:Cr	242	4.92	330,430,600
YAG:Fe	264	4.53	/

3.2. The measurement results $SrTiO_3$ and discussion

Strontium titanate is an ionic crystal of the perovskite structure known as a quantum paraelectric. The temperature dependence of the dielectric permittivity at temperatures below room temperature, and above 50 K is described by the Curie-Weiss dependence $\varepsilon_r(T) = C/(T-\theta)$, where C and θ are constants. At low temperatures (T < 50 K), permittivity deviates from the Curie –Weiss law, when the dependence of the dielectric permittivity can be approximated by Barrett's formula [18]. This discrepancy is explained by the existence of quantum fluctuations that prevent long-range order. Since the ferroelectric transition was not observed in quantum fluctuations, this crystal is known as quantum paraelectric. This study aims to examine the doping samples to determine whether deviations from their characteristic behavior exist.

Figure 3 shows the dependence of the dielectric permittivity $\varepsilon_r(T, f)$ as a function of temperature and frequency for undoped STO and doped STO:Ni, STO:Nd, STO:Sm crystals [4]. For all the studied samples, the value of dielectric permittivity gradually decreased as the temperature increased for all test frequencies and it can generally be described using the Curie-Weiss law which is in line with the results from the literature [19]. Also, it is noticeable that the temperature dependence was loosely related to the test frequencies. Further, in Figure 3b, the STO crystal doped by Ni ions showed a weak dependence of dielectric permittivity $SrTiO_3$ on temperature. A similar temperature dependence was observed in other crystals doped by 3d ions as described in [20,21]. The values of dielectric permittivity for all tested samples doped by 3d ions were lower than the corresponding values for the undoped STO.

Our measurements of the dependence $\varepsilon_r(T)$ for the undoped STO confirms the well-known fact from the literature that the existence of antiferodistorsion structural phase transition at 105 K does not lead to anomalies in the temperature dependence ε_r (T).

In contrast to the dependence, shown in Figures 3 (a) and (b), Figures 3 (c) - (d) show that there was a change in the speed of growth of the dielectric permittivity at temperatures below 120 K for the doped crystals 4f (Nd and Sm) ions. As the temperature fell, the permittivity gradually increased, and then there was a sudden growth at the temperature of about 120 K.

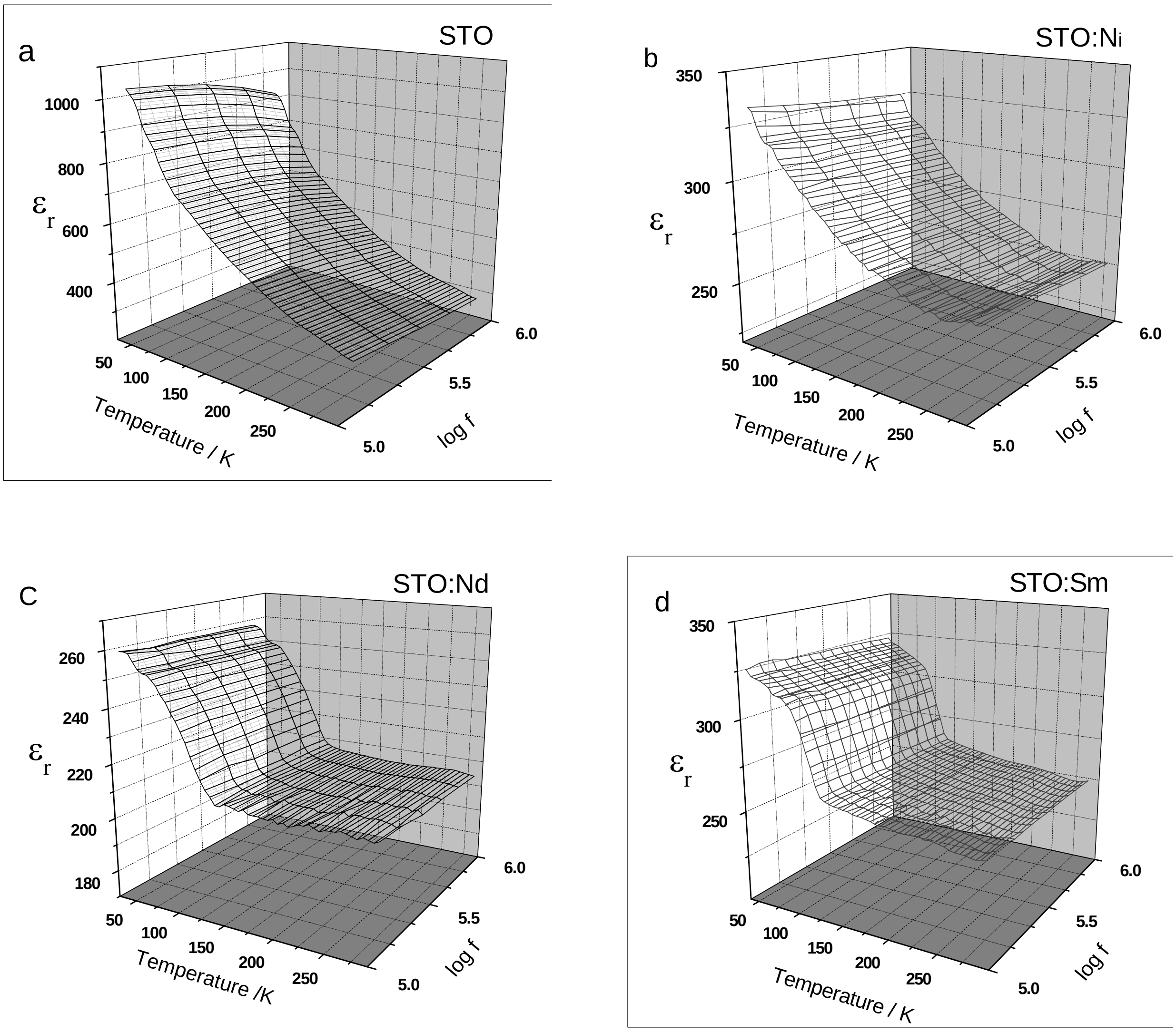


Figure 3. Dielectric permittivity as a function of temperature and frequency for (a) $SrTiO_3$*, (b)* $SrTiO_3$*:Ni, (c)* $SrTiO_3$*:Nd and (d)* $SrTiO_3$*:Sm monocrystals [4]*

To see the impact of doping by 4f - ions on dielectric characteristics more clearly, Figure 4 presents the inverse temperature dependence of the dielectric permittivity $\varepsilon_r^{-1}(T)$ for undoped and doped STO:Sm for test frequencies of 80 kHz, 2 MHz, 5 MHz, and 8 MHz [22]. There are two clearly observable fractures of the curve $\varepsilon_r^{-1}(T)$, one at the temperature around 90 K and the other at 120 K. The well-known structural phase transition actually belongs to the interval of 90 K – 120 K. In general, based on the previous measurements of dielectric characteristics it can be said that for the sample doped by 3d ions (Ni, Mn, V, Fe), there was a hardly noticeable fracture of inverse curve ε_r^{-1}(T) at the temperature close to the structural phase transition. In samples doped by the rare earth element, this fracture can be very clearly observed [22].

The difference between a subtle phase transition for STO crystal doped by 3d ions and clearly visible for STO crystal doped by 4f ions may indicate significant differences in the role that 3d and 4f ions have in the lattice of the STO.

In order to explain the origin of these differences, we conducted a detailed analysis from the point of the package of ions in the lattice of the perovskite crystals. Generally, to describe the stability of the perovskite structure, Goldsmith introduced the tolerance factor t. We consider that perovskite structure ABO_3 is tightly packed if the value tolerance factor is close to one. For STO crystal the value is 1.001, which places it in a group of ideal perovskite structures. The degree of packing of ions A or B in the perovskite lattice ABO_3 is well described by partial tolerance factors $t_1 = (r_A+r_O)/a$

and $t_2 = 2(r_B+r_O)/a$, where a is the lattice parameter, r_A, r_B and r_O are the radii of the corresponding ions [23]. The lattice parameter of the STO mono-crystals has a value of 0.3905 nm. On the basis of this approach when t_1 or $t_2<1$, ions A or B can fluctuate around their positions, while in the case where the t_1 or $t_2>1$, A or B ions are tightly packed [23].

Using the Valence shift method (VSXR), it was established that in almost all samples some part of the Ti^{4+} ions moved to the state of Ti^{3+}. The reasons for this change can be the crystal growth conditions, non-stoichiometry of the samples or a compensation of the charge. The biggest move, up to 20%, was observed in the samples doped by Sm and Nd ions [24]. Bearing in mind the electronic distribution of the zones in the case of the state of Ti^{3+}, one electron is in the 3d zone and thus the radius of Ti ions in the same environment is greater. This generally contributes to reducing the value of the tolerance factor and, therefore–to a greater rotation instability. Table 2 presents the estimated value of partial tolerance factor for 3d (V, Mn, Fe, Ni) and 4f (Nd, Sm, Er) ions [4]. Ion radii given in the table are the radii of ions for the assumed corresponding environment and the corresponding valence. 3d elements with coordination number 6 have a similar radius to the radius of Ti ions. The radius of Ti^{4+} ions in octahedral environment is 0.605Å. Taking into account the size of the radius of ion dopants and comparing with the radius of the ion lattice, it can be considered that 3d ions are likely to be implanted in the Ti^{4+} position in the perovskite crystals. For these ions, the calculated values of partial tolerance factor, t_2 are greater than 1. According to this value, 3d ions are firmly implanted in the grid $SrTiO_3$.

The valence of ions of rare earth oxides in the perovskite is usually 3+ [25]. Comparing the values of the radii, 4f-ion (Sm^{3+}, Nd^{3+}, Er^{3+}) are close to the radius of Sr^{2+} ions. The radius of Sr^{2+} in dodecahedron environment with coordination number 12 is 1.44 Å. These data suggest that the RE^{3+} ions during crystal growth will take position of ion A rather than B. In this case, RE^{3+} ion acts as a donor dopant necessitating a local charge compensation. Excess electrons can be affected by the Ti^{4+} ions which will be transformed to Ti^{3+} ions. Table 2 shows that the calculated partial tolerance factors t_1 of RE^{3+} ions are less than 1. This indicates that the 4f ions can fluctuate in the A position, which further suggests that the 4f ions are not so firmly embedded in the crystal lattice. Furthermore, the incorporation of rare earth ions in the STO lattice inter-ion RE-O distances differs from the distances Sr-O, which causes changes in the polarizability of ions also changing the shape of a regular octahedron TiO_6. On the other hand, TiO_6 octahedron plays an important role in the structural phase transition (T = 105 K). The angle φ of rotation of the octahedron TiO_6 is the primary parameter of aniferodistorsive phase transition order. The absence of fracture of the dielectric permittivity in dependence of temperature for samples doped by 3d ions could indicate that 3d doping has no significant impact on a network consisting of TiO_6 octahedrons.

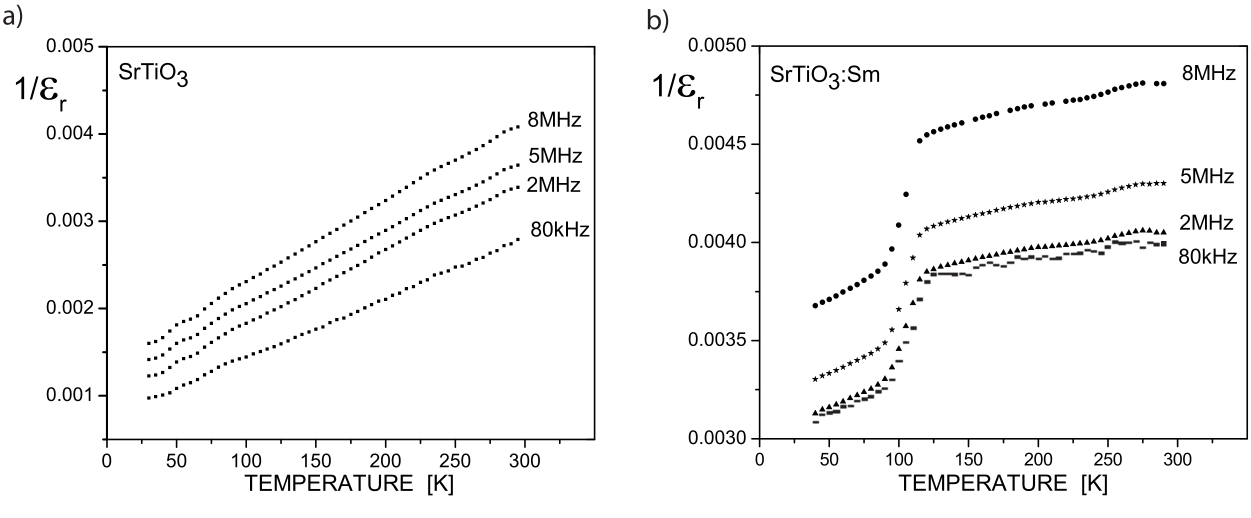


Figure 4. Inverse of dielectric permittivity (a) of pure $SrTiO_3$ *and (b)* $SrTiO_3$*:Sm crystal (test frequencies of 80 kHz, 2 MHz, 5 MHz and 8 MHz) [22]*

Table 2. Partial tolerance factors t_1 and t_2 for the 3d and 4f ions in the STO [4]

Ion	Coordination number	Valence	Ionic radii [Å]	Partial tolerance factor t_2	Partial tolerance factor t_1
Ti	VI	3+	0.67	1.06	
Ti	VI	4+	0.605	1.027	
V	VI	2+	0.79	1.121	
V	VI	4+	0.58	1.014	
Mn	VI	2+	0.67	1.060	
Fe	VI	2+	0.83	1.142	
Ni	VI	4+	0.53	0.99	
Ni	VI	2+	0.69	1.070	
Nd	VI	3+	0.98	1.220	
Sm	VI	3+	1.03	1.244	
Er	VI	3+	0.89	1.172	
Sr	XII	2+	1.44		1.025
Nd	XII	3+	1.27		0.967
Sm	XII	3+	1.24		0.956
Er	XII	3+	1.15		0.923

In addition to the dielectric measurements, the measurements in the UV - Vis and IC range were carried out. Without going into details, we would like to emphasize that there is a significant difference in the absorption spectra between samples of STO doped by 3d and 4f, which was analyzed in detail in paper [4].

4. CONCLUSION

This paper presents the results of studying the spectral and structural characteristics of the crystal $Y_3Al_5O_{12}$ (YAG), Al_2O_3 and $SrTiO_3$. Dielectric and optical properties of undoped YAG crystals and doped YAG:Ti, YAG:Cr and YAG:Fe crystals were compared. The results of UV-Vis spectra showed that the optical properties of YAG crystals are sensitive to the presence of dopants, which moved absorption edges, reduced the value of the energy gap and led to the emergence of new absorption peaks in the optical region of the spectrum. For YAG the obtained value of the energy gap was 6.91eV and for YAG doped by 3d ions (Ti, Cr, Fe) were 4.98 eV, 4.92 eV and 4.53 eV respectively. Within the test temperature and frequency range, the trend of the temperature dependence on the dielectric permittivity did not change significantly with the doped crystal as compared to the undoped ones. The deviation from dependence characteristic of ionic crystals and crystals with covalent bonds was observed for the temperatures above ambient ($T > 350$ K). Such a deviation was observed in all the doped samples. This can be explained by the diffusion of defects and ordering of stoichiometry of the samples.

The analysis of the dielectric measurements of STO crystals showed that in samples doped by 3d ions the Curie-Weiss law was valid for temperature greater than 50 K. For samples which were doped by ions 4f- the change observed was the increase of the dielectric permittivity with temperature decrease in the range about 80 –120 K. The temperature which corresponded to the temperature $T = 105$ K of the structural phase transition of $SrTiO_3$ was in the middle of this interval.

From the point of tolerance factors, 3d ions were implanted at the position Ti in the lattice of the STO. On the other hand, 4f ions replaced Sr ions and thereby influenced the mechanisms of dielectric polarization, especially near the antiferodistorsive phase transition at 105 K.

We can conclude that the dielectric and optical properties of the studied crystals depend on the type of doping ions and defects. Changes that occur can have an important impact on the performance of optical fiber devices, electronic memory devices, in magnetooptic and microwave engineering, and it is because of these numerous reasons they should be studied in more detail.

5. ACKNOWLEDGEMENT

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ПРОУЧАВАЊЕ СТРУКТУРНИХ И СПЕКТРАЛНИХ КАРАКТЕРИСТИКА ЛАСЕРСКИХ КРИСТАЛА $Y_3Al_5O_{12}$, Al_2O_3 И $SrTiO_3$ ДОПИРАНИХ 3d- И 4f- ЈОНИМА

Сажетак: Предмет проучавања наших истраживања су утицаји различитих третирања на структурне и спектралне карактеристике оксида ($Y_3Al_5O_{12}$, $SrTiO_3$ и Al_2O_3) који припадају групи јонских кристала са великим међузонским гепом. Проучаване су диелектричне и оптичке карактеристике ласерског монокристала итријум алуминијум граната $Y_3Al_5O_{12}$ (YAG), допираног јонима из групе гвожђа (3d-), монокристала Al_2O_3 и монокристала $SrTiO_3$ допираног 3d- и 4f- јонима. Због добрих физичких и оптичких карактеристика ласерски кристали YAG и Al_2O_3 и несвојствени параелектрик $SrTiO_3$ заузимају важно место у технологији и као такви имају велику примену. Диелектрична својства испитиваних монокристала су анализирана коришћењем диелектричне спектроскопије (80 kHz − 15 MHz) у широком температурском интервалу (50−400 K). Извршено је упоређивање температурских зависности диелектричне пропустљивости (ε_r) и диелектричних губитака (tanδ) за различите тест фреквенције за недопиране и допиране кристале. Оптичка својства су проучавана на основу апсорпционих спектара у UV-Vis региону. Експериментални резултати су показали да присуство 3d- допанта у YAG кристалу проузрокује померање апсорпционе ивице као и појаву карактеристичних пикова. Разлике које су уочене у апсорпционим спектрима највероватније су последица уграђивања 3d- јона на две могуће, симетријски различите позиције јона алуминијума, тетраедарске и октаедарске, у кристалној решетки YAG кристала. Проучавање спектралних карактеристика $SrTiO_3$ су показала да допирање 4f-јонима значајније утиче на структурне карактеристике $SrTiO_3$, посебно у близини структурног фазног прелаза који се дешава на температури око 105 K.

Кључне речи: $Y_3Al_5O_{12}$, $SrTiO_3$, допирање, диелектрична спектроскопија, UV-Vis спектроскопија.

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