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## STUDY OF THE INFLUENCE OF VARIATIONS IN THE PHASE COMPOSITION ON THE DIELECTRIC PROPERTIES OF FERROELECTRIC $\text{CaTiO}_3$ CERAMICS DOPED WITH $\text{Y}_2\text{O}_3$

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The study of the relationship between the effect of phase composition variation on the dielectric characteristics of ferroelectric ceramics is one of the most important fundamental questions, the answer to which will allow us to determine the potential of using ferroelectrics in microelectronic applications and the creation of alternative energy sources (solid oxide fuel cells). The purpose of this study is to explore the effect of the  $\text{Y}_2\text{O}_3$  dopant on the phase formation processes and the properties of the synthesized ferroelectric ceramics of calcium titanate, as well as to establish the connection between the influence of the formation of impurity phases on the change in the dielectric properties of ceramics. According to the data of X-ray phase analysis, it was found that the addition of  $\text{Y}_2\text{O}_3$  with a concentration above 0.15 M leads to the formation of an orthorhombic  $\text{CaY}_2\text{O}_4$  phase in the ceramic structure, the weight contribution of which increases with the dopant concentration growth. An analysis of the dependence of the specific electrical conductivity ( $\sigma_{\text{DC}}$ ) with varying dopant concentration showed that the maximum value of  $\sigma_{\text{DC}}$  is achieved at dopant concentrations of 0.05 M, which leads to structural ordering due to the effect of adding yttrium oxide acting as a stabilizer, as well as the formation of impurity donor conductivity in the structure. An analysis of the dependence of the specific electrical conductivity ( $\sigma_{\text{DC}}$ ) from dopant concentration was carried out. It has been established that the maximum value of  $\sigma_{\text{DC}}$  is achieved at a dopant concentration of 0.05 M. This is explained by structural ordering due to the addition of a stabilizer – yttrium oxide, as well as the formation of impurity donor conductivity in the synthesized sample. At the same time, the established dependences of the change in dielectric characteristics are in good agreement with the change in the phase composition, and an increase in the concentration of charge carriers due to the introduction of a donor impurity in the form of  $\text{Y}^{3+}$  leads to the appearance of volume-charge polarization in ceramics.

**Keywords:** ferroelectrics, doping, phase transformations, mechanochemical synthesis, dielectrics.

### INTRODUCTION

Today, much attention in the world is paid to expanding the range of practical applications of various ferroelectric ceramics with a perovskite or perovskite-like structure in microelectronic applications, in particular, in the creation of piezoelectric devices, resonators, ultrasonics, integrated circuits, capacitors or anode materials for solid oxide fuel cells. Interest in these types of ceramics is due to their high dielectric characteristics, which can ensure the creation of high-precision devices with a low level of dielectric losses, as well as high resistance to external influences, including large temperature fluctuations, mechanical stress, etc. [1–3, 8–12]. At the same time, among the variety of ferroelectric ceramics, structures of the  $\text{ABO}_3$  type occupy a special place, where A – are rare-earth or alkali elements, B – transition metal elements. In this case, each B cation is surrounded by O anions, while the A cation occupies more advantageous positions at the sites [4, 5]. Interest in these types of structures is primarily due to their ferroelectric characteristics, which can form dipoles when exposed to external forces (mechanical pressure or electric fields). At the same time, in the case of external influences, the resulting dipoles are able to change their orientation, which in turn leads to the appearance of polarization effects and electric charges [6, 7]. Under the

influence of external forces, the dipoles are reoriented. That causes a change in polarization and the creation of an additional charge, which enhances efficiency [8–12].

The aim of this work is to establish the relationship between the variation in the phase composition with a change in the concentration of the  $\text{Y}_2\text{O}_3$  dopant in the composition of ferroelectric ceramics based on calcium titanate ( $\text{CaTiO}_3$ ), as well as its effect on the dielectric properties of ceramics. The choice of ceramics based on  $\text{CaTiO}_3$  as objects of study is due to the prospects of using them as anode materials for solid oxide fuel cells, as well as the basis for creating capacitors, due to the high dielectric constant and low dielectric losses. At the same time, doping with yttrium oxide ( $\text{Y}_2\text{O}_3$ ) will not only solve the problem of accelerating the processes of phase transformations, but also at high concentrations will make it possible to create two-phase ceramics, the formation of which enables to influence the change in dielectric characteristics. As shown earlier in [13–15], the use of the mechanochemical synthesis method to obtain ferroelectric ceramics based on titanates is accompanied by the formation of impurity inclusions in the form of titanium dioxide (in the form of anatase or rutile phases), which has a significant effect on the dielectric properties of ceramics. Precipitation of inclusions in the form of impurity phases of anatase or rutile

(the formation of which occurs as a result of the initialization of polymorphic transformations) is primarily due to insufficient sintering temperature (annealing was carried out at a temperature of 1000–1300 °C). In this case, the use of  $\text{Y}_2\text{O}_3$  as a dopant will make it possible to avoid the formation of impurities in the form of inclusions of titanium dioxide phases, as well as to increase the degree of structural ordering.

#### MATERIALS AND METHODS

Synthesis of ferroelectric ceramics based on calcium titanate doped with yttrium oxide was carried out using the method of mechanochemical synthesis followed by thermal annealing of the resulting mixture.  $\text{CaCO}_3$ ,  $\text{TiO}_2$  (anatase),  $\text{Y}_2\text{O}_3$  were chosen as the initial components of the powders. The chemical purity of the initial components was 99.95%, purchased from Sigma Aldrich (Sigma, St. Louis, Missouri, USA). The  $\text{Y}_2\text{O}_3$  dopant concentration was chosen from 0.05 to 0.25 M. The synthesis of selected mixtures after grinding was subjected to thermal annealing at a temperature of 1300 °C for 5 hours, followed by cooling inside a muffle furnace (Snol, Lithuania) for 24 hours to eliminate the effects associated with hardening and the formation of oxides or nonequilibrium inclusions.

The phase composition of ceramics was determined via the X-ray phase analysis method implemented using a D8 Advance ECO X-ray diffractometer (Bruker, Germany). X-ray diffraction patterns were taken in the Bragg-Brentano geometry in the angular range  $2\theta = 20\text{--}90^\circ$ , with a step of  $0.03^\circ$ . The DiffracEVA v.4.2 software was used to determine the phases and refine the structural characteristics (lattice parameters and volume). The refinement of the parameters was carried out by a comparative analysis with the card values of the standards from the PDF-2 database (2016). The phase ratio was determined by comparative analysis of the areas of diffraction

reflections for each established phase, followed by determination of the weight contribution of each phase.

The measurement of porosity was carried out on the basis of changes in the structural parameters of the crystal lattice and its volume, taking into account the variation in the molecular weight of the samples. This technique is one of the simplest for determining the porosity of ceramics.

The dielectric properties of the synthesized samples were measured on pressed tablets, for the preparation of which a binder was first introduced from a solution of polyvinyl alcohol with water. The pressing of powders with a binder was carried out in a hydraulic press (Sorokinstrument, Russia) with a maximum load of 200 MPa. Next, the tablets were dried in an oven at 60°C to remove moisture. The dry residue of polyvinyl alcohol in pressed tablets was no more than 5% by weight. The measurement of the frequency spectra of the capacitance and the dielectric loss tangent in the frequency range of 2–200 000 Hz at room temperature was carried out on a HIOKI IM3533-01 impedance meter by applying silver paste on the surface of the tablets. The permittivity value was made through recalculation according to the capacitance formula of a flat parallel capacitor.

#### RESULTS AND DISCUSSION

Figure 1 shows the results of X-ray diffraction of the studied ceramics with the perovskite structure, obtained at different concentrations of the  $\text{Y}_2\text{O}_3$  dopant and without the addition of that of. Also, for comparison and determination of the main structural and phase changes, an X-ray diffraction pattern of perovskite ceramics obtained without the addition of a  $\text{Y}_2\text{O}_3$  dopant is presented. According to the X-ray analysis, it was found that in the initial state, the ceramics obtained are the structure of perovskite  $\text{CaTiO}_3$  with an orthorhombic crystal lattice, spatial syngony  $Pbnm(62)$ .

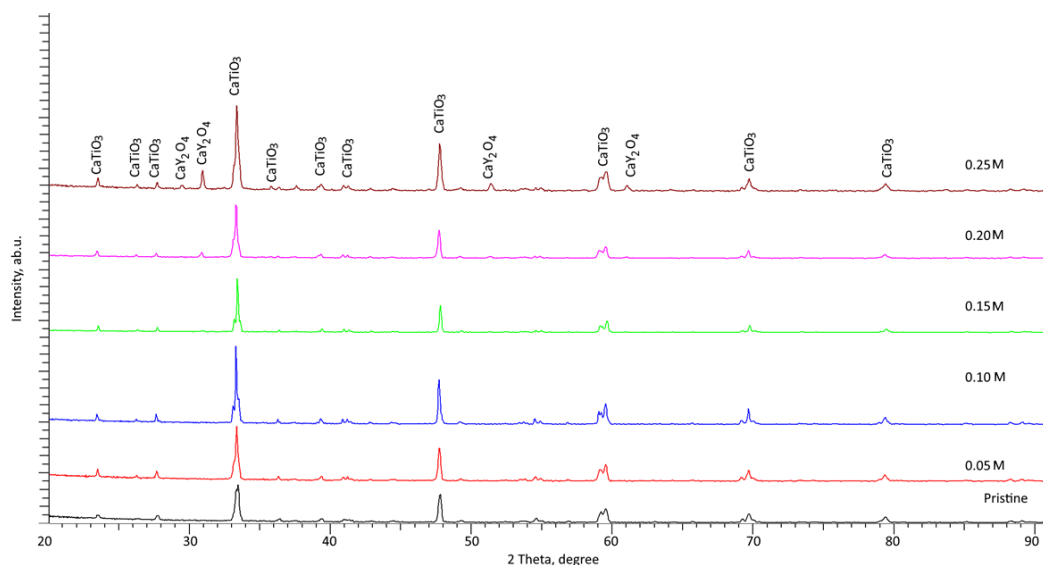


Figure 1. Results of X-ray diffraction of the studied perovskite ceramics depending on the change in the  $\text{Y}_2\text{O}_3$  dopant concentration

At the same time, an analysis of the shape and position of the diffraction lines showed that the observed sample does not contain any impurity phases or inclusions, which indicates the complete completion of the processes of phase formation of the perovskite structure under the selected conditions of thermal annealing. An estimate of the symmetry degree of the X-ray reflections for the observed phase showed that the structure of the samples contains defective inclusions and regions of disorder, the presence of which is confirmed by the asymmetry of the diffraction reflections with respect to the position of the maximum.

In the case of doping with  $\text{Y}_2\text{O}_3$  at a concentration of 0.05–0.10 M, was observed. This implies the defective fraction reduction and the crystallinity degree growth. At the same time, the appearance of new diffraction reflections for this range was not established, which indicates that at the given concentrations of the  $\text{Y}_2\text{O}_3$  dopant, the processes of phase transformations or the formation of new structural inclusions do not occur, or the content of new inclusions is less than 1%, which cannot be identified. In turn, changes in the shape of diffraction reflections, as well as changes in the position of the maxima, indicate that the addition of  $\text{Y}_2\text{O}_3$  results in structural ordering in the ceramic structure, which is manifested in a decrease in the concentration of the defect fraction and an increase in the crystallinity degree.

At a  $\text{Y}_2\text{O}_3$  dopant concentration of 0.15 mol, low-intensity diffraction reflections are observed in the region  $2\theta = 32\text{--}33^\circ$  and  $52\text{--}54^\circ$ , which are characteristic of the  $\text{CaY}_2\text{O}_4$  orthorhombic phase of the  $Pbnm(62)$  spatial system, the formation of which is due to the processes of structural and phase transformations when titanium is replaced by yttrium, followed by the formation of a new phase inclusion. At the same time, the assessment of the contribution of this phase showed that its content is no more than 5%, and the sizes of these inclusions are no more than 15–20 nm, with grain sizes of the main phase of 50–60 nm.

General conclusions about the observed changes in phase transformations can be formulated as follows. An analysis of phase changes in the composition of ferroelectric perovskite ceramics with an increase in the  $\text{Y}_2\text{O}_3$  dopant concentration showed that, at a dopant concentration of more than 0.10 M, the formation of an orthorhombic  $\text{CaY}_2\text{O}_4$  phase occurs, the concentration of which increases from 5% to 20% with an increase in concentration from 0.15 M to 0.25 M. At the same time, the formation of the  $\text{CaY}_2\text{O}_4$  phase leads to compaction of the ceramic structure due to a decrease in porosity, as well as an increase in the degree of structural ordering. On the basis of a calculated estimate of the weight contributions of each established phase, a phase diagram was constructed reflecting changes in the phase ratio depending on the variation in the  $\text{Y}_2\text{O}_3$  dopant concentration. The results of these calculations are shown in Figure 2a.

During the studies carried out, the phase transformation processes in ferroelectrics upon doping with  $\text{Y}_2\text{O}_3$

can be written as follows:  $\text{CaTiO}_3 \rightarrow \text{CaTiO}_3/\text{CaY}_2\text{O}_4$ . It should be noted that the formation of two-phase ceramics is observed at a dopant concentration above 0.15 mol, which indicates that the yttrium content in the composition must be very high for the formation of the orthorhombic  $\text{CaY}_2\text{O}_4$  phase. The formation of the  $\text{CaY}_2\text{O}_4$  phase, depending on the increase in the dopant concentration from 0.15 to 0.25 M, obeys an almost linear law, which indicates the possibility of controlled synthesis of ceramics with a given concentration of the impurity phase.

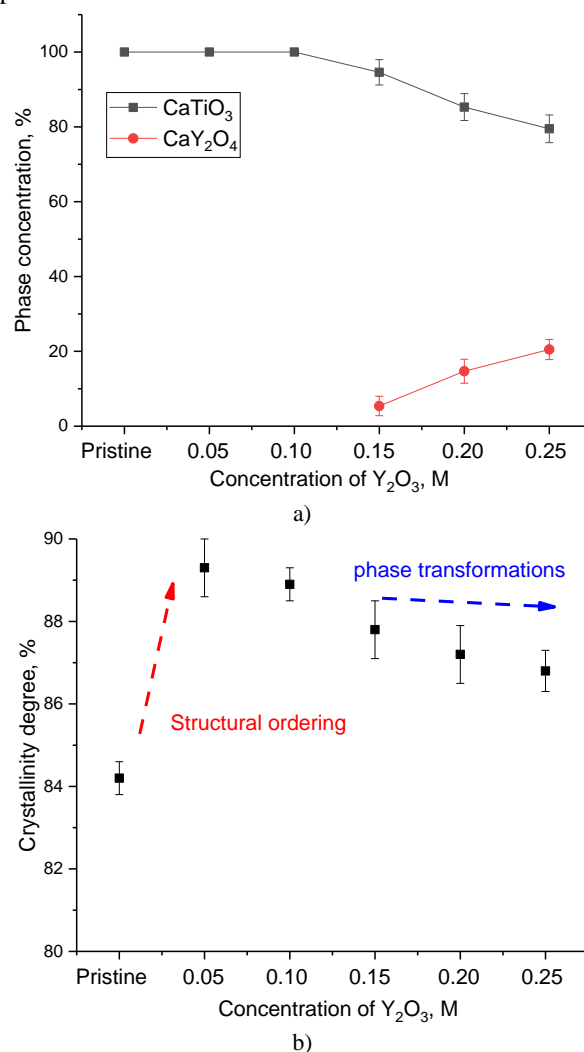


Figure 2. Diagram of the phase composition in ferroelectric ceramics with varying  $\text{Y}_2\text{O}_3$  dopant concentration (a) and results of the alteration in the structural ordering degree (crystallinity degree) of ceramics depending on the  $\text{Y}_2\text{O}_3$  dopant concentration (b)

The data on changes in the structural ordering degree (crystallinity degree) presented in Figure 2b reflect the positive effect of the addition of the  $\text{Y}_2\text{O}_3$  dopant on the decrease in the concentration of defective inclusions in the composition of ceramics at low dopant concentrations (0.05–0.10 M). In this case, two characteristic regions can be distinguished, corresponding to different types of

structural changes. The first region is typical for dopant concentrations of 0.05–0.10 M, and corresponds to an increase in the degree of structural ordering associated with the compaction of ceramics and a decrease in the concentration of defective inclusions and residual stresses caused by mechanochemical grinding and subsequent annealing. The second region is typical for dopant concentrations above 0.15 M, for which a new phase is formed. At the same time, annealing with the addition of a  $\text{Y}_2\text{O}_3$  dopant concentration leads to a more intense ordering of the structure in comparison with undoped ceramics annealed at the same temperature. In this case, it is possible that the addition of  $\text{Y}_2\text{O}_3$  at low concentrations to the composition leads to an acceleration of the processes of structural ordering during thermal annealing due to a change in the magnitudes of thermal vibrations of the crystal lattice, as well as the filling of vacancy positions. At  $\text{Y}_2\text{O}_3$  dopant concentrations above 0.15 mol, which are characterized by the formation of  $\text{CaY}_2\text{O}_4$  phase inclusions, a slight decrease in the degree of structural ordering is observed, the decrease of which is inversely proportional to the increase in the weight contribution of the  $\text{CaY}_2\text{O}_4$  phase in the composition of ceramics. Such a decrease can be explained by the effects associated with the deformation of the structure due to the increase in interfacial boundaries with a rise in the  $\text{CaY}_2\text{O}_4$  content contribution.

Based on the obtained X-ray diffraction patterns, the structural parameters were calculated, the dynamics of which reflects the effect of the dopant on the deformation distortion of the crystal lattice. Table 1 presents data on changes in the parameters and volume of the crystal lattice of perovskite ceramics depending on the  $\text{Y}_2\text{O}_3$  dopant concentration.

As can be seen from the data, in the case of varying the concentration of the  $\text{Y}_2\text{O}_3$  dopant from 0.05 to 0.10 M, a decrease in the parameters of the crystal lattice, as well as its volume, is observed, which indicates the structural ordering of the ceramics and the perfection of the crystal lattice. This leads to an increase in the density of ceramics due to its compaction with a partial decrease in deformation distortions and residual stresses that have arisen during mechanochemical grinding. In this case, the  $\text{Y}_2\text{O}_3$  dopant acts as a stabilizing additive, which is used to accelerate the processes of structural ordering during thermal sintering [16, 17]. During the formation of the

$\text{CaY}_2\text{O}_4$  phase in the case of concentrations of 0.15–0.20 M, the volume of the crystal lattice becomes denser and its structural parameters decrease, which indicates a decrease in deformation distortions in the ceramic composition. However, in the case of a dopant concentration of 0.25 M, a slight increase in the lattice volume is observed, which may be due to the effects of interfacial boundaries, leading to volume deformation.

Figure 3 shows the dependences of the real part of the permittivity  $\epsilon'$  and the dielectric loss tangent for the obtained composites. The obtained values of the permittivity and loss tangent clearly indicate the dielectric properties of the obtained samples. As can be seen from Figure 1a, the permittivity value  $\epsilon'$  decreases with the frequency  $f$  growth. This is due to the delay in following the electric charges in ceramics, which contribute to the polarization, behind the alternating field. In the low-frequency region, interfacial polarization, ion hopping polarization (displacement of polarons, point defects) can contribute to the polarization. This dependence is well described by the Debye relaxation model [18]. In the high-frequency region, the value of  $\epsilon'$  decreases due to the contribution of only the ionic and dipole orientational polarizations. The measured value of  $\epsilon'$  of pure  $\text{CaTiO}_3$  is less than reported in other works [19–21]. This is due to the powder form of ceramics and the imperfection of the crystal structure. The pronounced frequency dependence of the dielectric permittivity in the frequency range of 2–300 Hz for samples with a dopant concentration of 0.05, 0.10 mol is associated with volume-charged polarization in a heterogeneous medium at the grain-with-semiconducting properties/dielectric grain boundary interface (Maxwell-Wagner mechanism) [22]. An increase in grain conductivity is associated with the incorporation of  $\text{Y}^{3+}$  ions into the B position of the perovskite crystal lattice with the substitution of the  $\text{Ti}^{4+}$  ion and the formation of a donor pair, as a result of which the concentration of charge carriers grows [21].

The frequency dependences of the dielectric loss tangent (see the data in Figure 3b) indicate that the decrease in the value of  $\tan \delta$  with increasing frequency is also associated with polarization processes. When the polarization mechanisms are switched off, the energy dissipation due to charge reorientation decreases with increasing  $f$ , which reduces the value of  $\tan \delta$  [23].

Table 1. Structural parameter data

Phase		Y <sub>2</sub> O <sub>3</sub> dopant concentration, M					
		0	0.05	0.10	0.15	0.20	0.25
<b>CaTiO<sub>3</sub> – Orthorhombic</b>	Crystal lattice parameter, Å	a=5.4008, b=7.6203, c=5.3607	a=5.3943, b=7.6052, c=5.3564	a=5.3868, b=7.5981, c=5.3521	a=5.3709, b=7.5876, c=5.3385	a=5.3742, b=7.6189, c=5.3521	a=5.3784, b=7.6249, c=5.3563
	Crystal lattice volume, Å <sup>3</sup>	220.33	219.71	219.06	217.56	219.14	219.67
<b>CaY<sub>2</sub>O<sub>4</sub> – Orthorhombic</b>	Crystal lattice parameter, Å				a=5.3742, b=7.6189, c=7.6843	a=5.3602, b=5.6454, c=7.6647	a=5.3465, b=5.6432, c=7.6572
	Crystal lattice volume, Å <sup>3</sup>				232.95	321.94	231.03

In the low-frequency region for the 0.05 mol sample, high dielectric losses are also associated with through conduction in ceramics due to the influence of  $\text{Y}^{3+}$  impurity ions. The difference in the values of the permeability, dielectric loss tangent, in addition to the influence of the alloying component and phase composition, is also associated with the morphology of the powder particles and ceramic porosity.

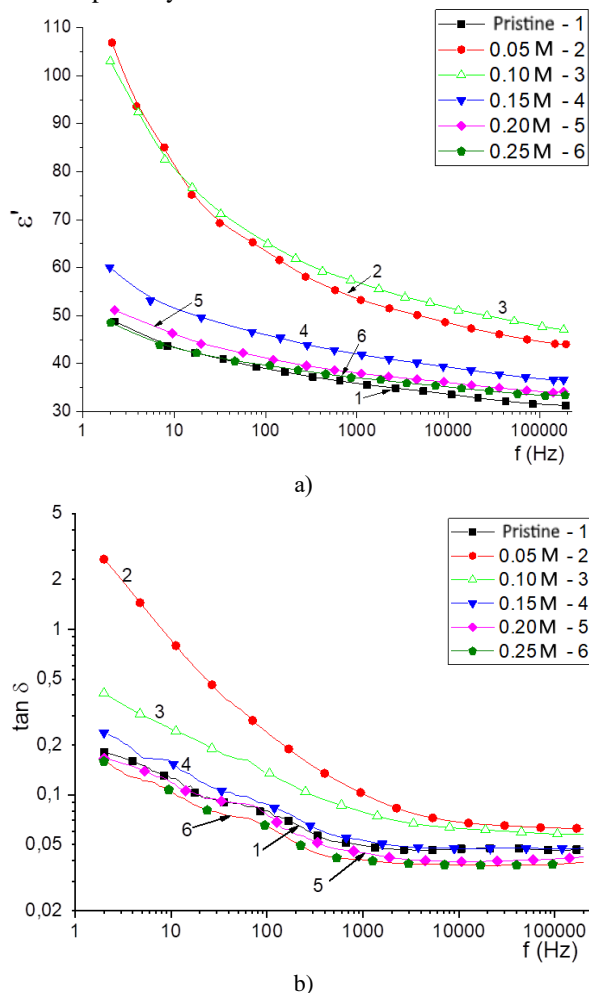


Figure 3. Frequency dependences of the real part of the permittivity (a) and the dielectric loss tangent (b) of the obtained samples

Figure 4a shows the dependences of the dc electrical conductivity  $\sigma_{DC}$  on the dopant concentration. It can be seen that the dependence passes through a maximum, which is due to the influence of impurity donor conductivity. When the concentration exceeds 0.15 M, the electrical conductivity decreases, which is associated with the formation of a new  $\text{CaY}_2\text{O}_4$  phase, which reduces the doping effect in  $\text{CaTiO}_3$ . The through conductivity of grains can also be judged from the Cole-Cole dependences  $-Z''(Z')$  in Figure 4b. It can be seen that only for the 0.05 M sample, the dependence  $Z''(Z')$  has the form of a semicircle, while for other samples this dependence is a straight line. This indicates the mechanism of current flow through grains with semiconductor properties [24].

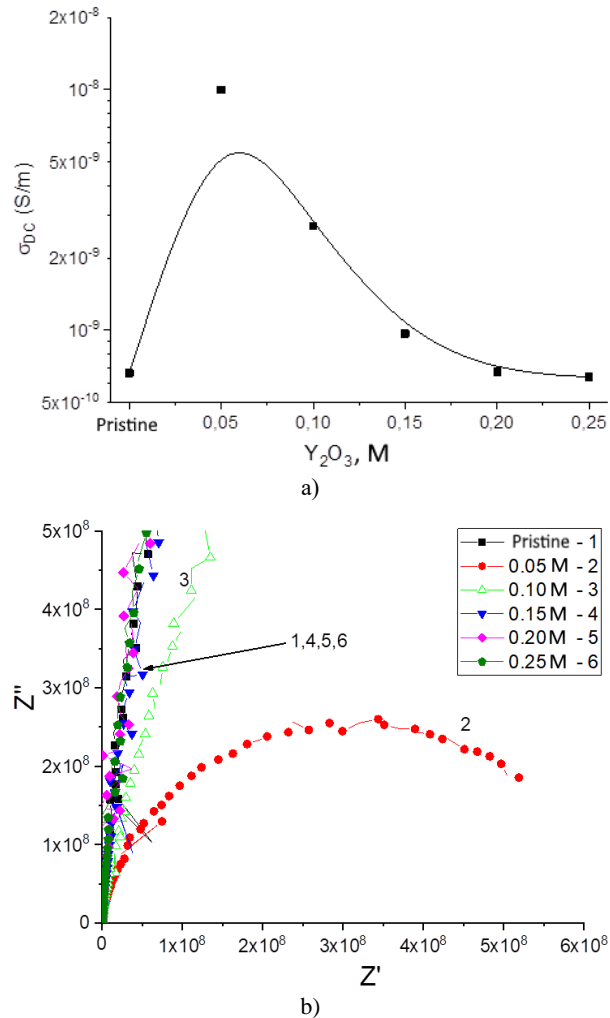


Figure 4. Dependence of the electrical conductivity at direct current on the concentration of the dopant (a) and the Cole-Cole diagram (b) of the obtained samples

From Table 2, it can be seen that the value of  $\epsilon'$  in the low frequency range varies from 43.32 to 81.64, while in the high frequency range from 33.59 to 51.83. The pronounced increase in the permittivity, in addition to the reasons described above, is also associated with an improvement in the crystal structure in the  $\text{CaTiO}_3$  phase.

Table 2. Comparison of permittivity  $\epsilon'$ , dielectric dissipation tangent  $\tan \delta = \epsilon''/\epsilon'$  at 10 Hz, 10 000 Hz and DC electrical conductivity  $\sigma_{DC}$

Concentration of $\text{Y}_2\text{O}_3$ , M	$\epsilon'$ (10 Hz)	$\epsilon'$ (10 000 Hz)	$\tan \delta$ (10 Hz)	$\tan \delta$ (10 000 Hz)	$\sigma_{DC} \cdot 10^{-10}$ , S/m
0.00	43.38	33.59	0.13	0.047	6.65
0.05	81.64	48.49	0.93	0.068	99.70
0.10	81.00	51.83	0.26	0.063	27.2
0.15	51.57	39.26	0.12	0.047	9.70
0.20	46.07	36.02	0.12	0.040	6.70
0.25	43.32	35.08	0.10	0.038	6.40

It should be noted that the values of the high-frequency permittivity of the doped samples are higher than those of the original  $\text{CaTiO}_3$ . This can be related to the fact that some entry of  $\text{Y}^{3+}$  ions into grains of the perovskite phase is realized, which increases the value of the high-frequency  $\varepsilon'$ . Similar results were obtained in studies on doping  $\text{MgTiO}_3$  with  $\text{Fe}^{3+}$  and  $\text{Cr}^{3+}$  ions at a concentration of 1 at.% [25]. The dependences of the concentration of dielectric characteristics correlate with the change in dc conductivity, which may indicate the dominant effect of electrical conductivity processes on the dielectric properties of the resulting ceramics.

## CONCLUSION

The paper presents the results of studies of the effect of  $\text{Y}_2\text{O}_3$  doping on the change in the phase composition, structural parameters, and dielectric characteristics of synthesized ceramics based on calcium titanate. Ceramics were obtained using mechanochemical solid-phase synthesis followed by thermal sintering of the resulting powders at a temperature of 1300 °C. During the studies, it was found that the addition of  $\text{Y}_2\text{O}_3$  at low concentrations of 0.05–0.10 M leads to an increase in the degree of structural ordering, and at concentrations above 0.15 M, inclusions are formed in the form of an orthorhombic  $\text{CaY}_2\text{O}_4$  phase, the weight contribution of which increases in direct proportion to the change in dopant concentration. Impedance spectroscopy on the obtained samples revealed that the synthesized ceramic powders are dielectrics with the value of  $\varepsilon'$  in the low-frequency region in the range from 43.32 to 81.64, and in the high-frequency region in the range from 33.59 to 51.83. Alterations in the dielectric characteristics ( $\varepsilon'$ ,  $\tan \delta$ ) as a function of the  $\text{Y}_2\text{O}_3$  concentration correlate with changes in the electrical conductivity, which is associated with the doping of  $\text{CaTiO}_3$  with  $\text{Y}^{3+}$  ions. At the same time,  $\text{Y}^{3+}$  is a donor impurity, which increases the concentration of charge carriers and causes a pronounced volume-charge polarization in ceramics. In addition, the dielectric properties depend on the imperfection of the crystal structure, the morphology of ceramic particles.

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## **$\text{Y}_2\text{O}_3$ ДОПИРЛЕНГЕН $\text{CaTiO}_3$ ФЕРРОЭЛЕКТРЛІК КЕРАМИКАЛАРЫНЫҢ ФАЗАЛЫҚ ҚҰРАМНЫҢ ВАРИАЦИЯСЫНЫҢ ДИЭЛЕКТРЛІК ҚАСИЕТТЕРІНЕ ӘСЕРІН ЗЕРТТЕУ**

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Фазалық құрамның вариациясының ферроэлектрлік керамиканың диэлектрлік сипаттамаларына әсерінің өзара байланысын зерттеу, ең маңызды іргелі сұрақтардың бірі болып табылады, оның жауабы микроэлектрондық қосымшаларда ферроэлектриктерді қолдану және баламалы энергия көздерін (қатты оксидті отын элементтері) құру әлеуетін анықтауға мүмкіндік береді. Бұл зерттеудің мақсаты –  $\text{Y}_2\text{O}_3$  допантының фазалық түзілу процестеріне және синтезделген кальций титанаты ферроэлектрлік керамикаларының қасиеттеріне әсерін зерттеу, сонымен қатар керамиканың диэлектрлік қасиеттерінің өзгеруіне қоспа фазаларының пайда болуының әсерін анықтау. Рентгендік фазалық талдау деректеріне сәйкес концентрациясы 0,15 мольден жоғары  $\text{Y}_2\text{O}_3$  қосылуы құрылымда  $\text{CaY}_2\text{O}_4$  орторомбиялық фазасының керамикасының пайда болуына әкелетіні анықталды, оның салмақтық үлесі допант концентрациясының жоғарылауымен артады. Допант концентрациясының вариациясындағы меншікті электр өткізгіштігінің ( $\sigma_{\text{DC}}$ ) тәуелділігін талдау  $\sigma_{\text{DC}}$  максималды мәніне допанттың 0,05 моль концентрациясында қол жеткізілетінін көрсетті, бұл тұрақтандырғыш ретінде әрекет ететін иттрий оксидін қосу әсеріне, сондай-ақ құрылымдағы қоспа донорлық өткізгіштіктің қалыптасуына байланысты құрылымдық ретке келтіруге әкеледі. Бұл ретте диэлектрлік сипаттамалардың өзгеруінің белгіленген тәуелділіктері фазалық құрамның өзгеруімен сәйкес келеді, ал  $\text{Y}^{3+}$  түрінде донорлық қоспаны енгізуге байланысты заряд тасымалдаушылардың концентрациясының артуы керамикада көлемдік зарядтау поляризациясының пайда болуына әкеледі.

**Түйін сөздер:** ферроэлектриктер, допирлеу, фазалық ауысулар, механохимиялық синтез, диэлектриктер.

## **ИССЛЕДОВАНИЕ ВЛИЯНИЯ ВАРИАЦИИ ФАЗОВОГО СОСТАВА НА ДИЭЛЕКТРИЧЕСКИЕ СВОЙСТВА СЕГНЕТОЭЛЕКТРИЧЕСКИХ КЕРАМИК $\text{CaTiO}_3$ ДОПИРОВАННЫХ $\text{Y}_2\text{O}_3$**

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Изучение взаимосвязи влияния вариации фазового состава на диэлектрические характеристики сегнетоэлектрических керамик является одним из наиболее важных фундаментальных вопросов, ответ на который позволит оптимизировать потенциал применения сегнетоэлектриков в микроэлектронных приложениях и создании альтернативных источников энергии (твердооксидных топливных элементов). Целью данного исследования является изучение влияния допанта  $\text{Y}_2\text{O}_3$  на процессы фазообразования и свойства синтезированных сегнетоэлектрических керамик титаната кальция, а также установление взаимосвязи влияния формирования примесных фаз на изменение диэлектрических свойств керамик. Согласно данным рентгенофазового анализа установлено, что добавление  $\text{Y}_2\text{O}_3$  с концентрацией выше 0,15 моль приводит к формированию в структуре керамик орторомбической фазы  $\text{CaY}_2\text{O}_4$ , весовой вклад которой увеличивается при увеличении концентрации допанта. Анализ зависимости удельной электропроводности ( $\sigma_{\text{DC}}$ ) при вариации концентрации допанта показал, что максимальное значение

$\sigma_{\text{DC}}$  достигается при концентрациях допанта 0,05 моль, приводящей к структурному упорядочению, обусловленному эффектом добавления оксида иттрия выступающим в качестве стабилизатора, а также формированием в структуре примесной донорной проводимости. При этом установленные зависимости изменения диэлектрических характеристик имеет хорошее согласие с изменением фазового состава, а увеличение концентрации носителей заряда, обусловленное внедрением донорной примеси в виде  $\text{Y}^{3+}$  приводит к возникновению объемно-зарядной поляризации в керамики.

**Ключевые слова:** сегнетоэлектрики, допирование, фазовые превращения, механохимический синтез, диэлектрики.