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The dependence of electrical conductivity of $Mg_xZn_{1-x}O$ ceramics on phase composition

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Abstract. The structural and electrical characteristics of (Mg,Zn)O ceramics produced using the solid state reaction at 1100 °C for 3 hours were studied applying X-ray diffraction and IR reflection spectroscopy as well as means of direct current measurements *versus* MgO content in initial charge (varied from 0 to 100 mol.%). It has been shown that electrical conductivity extracted from the IR reflection spectra corresponds to that of hexagonal phase in a solid solution, while plasmon in cubic phase was not observed. The electron concentration in the hexagonal grains of solid solution prepared with MgO content below 30 mol. % in the charge was found to be close to that of ZnO grains. It shows the tendency to decrease with further growth of the MgO content, which was explained by extraction of zinc interstitials, responsible for ZnO conductivity, from ZnO under formation of the MgZnO cubic phase. The direct current measurements have shown the lower conductivity as compared to the value estimated from IR reflection spectra. This fact along with the superlinearity of current-voltage characteristics has been explained by the presence of intergranular barriers, which does not allow obtaining information on the concentration of free electrons in the grain by this method. The possible nature of intergranular barriers as well as the role of grain boundaries in the DC conductivity of samples has been discussed.

Keywords: MgZnO ceramics, X-ray diffraction, electrical conductivity, IR reflection spectroscopy.

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1. Introduction

Zinc oxide exhibits a number of unique properties that determines its high potential for applications in electronics, medicine, photonics, various sensors and radiation detectors (specifically, for development of different types of photodetectors, light emitting devices, varistors, gas sensors, catalysts, *etc.*) [1]. This semiconductor is a non-toxic and relatively inexpensive material of *n*-type conductivity with direct wide band gap (E_g = 3.37 eV at 300 K), a large exciton binding energy (60 meV) [1], high mechanical and thermal stability, chemical and radiation resistance.

To increase the band gap and the sensitivity of ZnO in the ultraviolet range of spectrum, its doping with magnesium is used. This also leads to a change in the value of electrical conductivity, and in the films of solid solutions obtained by different methods, as well as in pressed nanopowders and ceramics, its reduction is usually observed [2–6]. However, there are also reports on an increase in the conductivity of magnesium doped ZnO ceramics [7].

At the same time, the reasons for the decrease in the electrical conductivity of (Mg,Zn)O solid solutions, and even more of its increase, with increasing magnesium content are still unclear, and information on the nature of intrinsic defects in solid solution, their concentration and position of their energy levels is insufficient. In particular, it was assumed that the decrease in conductivity may be caused by a decrease in the concentration of interstitial zinc due to increased energy of its formation [2, 3], increasing depth of donor energy level [4], self-compensation processes (zinc vacancies formation [5]), structural defects in crystallites [6], decrease in electron mobility [4], as well as by the appearance of pores [2, 8]. At high Mg concentrations, the decrease in conductivity was also assigned to the appearance of inclusions of the (Mg,Zn)O cubic phase [6].

Note that most of the works were performed on polycrystalline films of solid solutions (including the textured ones) and measured using the direct current method. These films often exhibit the presence of barriers at the crystallite boundaries, in particular, due to the adsorption of oxygen on their surface, which leads to formation of electron-depleted regions. This phenomenon was observed in textured ZnO films prepared using magnetron sputtering [9] and consisted of ZnO columns. The same effect can also be caused by the appearance of pores, the number of which can increase with increasing magnesium content [2]. It should be also noted that the adsorption of atoms that capture electrons of crystallites can lead to a decrease in the conductivity of the entire volume of crystallites, if the size of depletion region is close to their sizes [9]. Thus, if the barriers are present in the sample, the direct current (DC) conductivity will not reflect the conductivity of grains.

The ceramic samples are also polycrystalline and the decrease of DC conductivity with Mg doping can be also caused by presence of barrier. However, in ceramic samples a decrease in the value of alternating current (AC) conductivity with increasing the magnesium content was observed [10]. In this case, the model of the hopping correlated barrier and the overlapping large polaron tunneling models were considered as a conduction mechanism [10].

It should be noted that ceramics consist of a mixture of grains with the hexagonal and cubic phases of solid solution, the conductivity of which can differ significantly. In this case the DC conductivity can depend on ceramic structure, in particular, on the contacts between the grains of different phases, which depend on MgO content. For example, it can be defined by lower-impedance grains, if there is a direct contact between them. Besides, measurements of both DC and AC conductivity do not enable to determine which phase is responsible for the measured conductivity.

Thus, the study of the reasons of conductivity decrease in zinc oxide doped with magnesium requires further research. In particular, it is necessary to separate the possible influence of barriers on the sample conductivity and define the carrier concentration in the grains. A convenient method for this is to study the spectra of specular infrared (IR) reflection, which allows determining the electrical parameters of grains from analysis of their plasma subsystem. The comparison of the obtained data with the results of DC conductivity measurements, including temperature dependence and current-voltage characteristics, can discover the presence of barriers. This method has been successfully used to determine the electrical characteristics of single crystals and textured ZnO films [9]. Besides, the comparison of measured carrier concentration with the contribution of grains of different phases can clarify the role of each phase in electrical conductivity.

In this work, the structural characteristics of (Mg,Zn)O ceramic samples with different magnesium content and specular IR reflection spectra were studied, and the electrical parameters of ceramic grains determined from their analysis were compared with the data obtained from DC measurements.

2. Experimental details

(Mg,Zn)O ceramics with different MgO content (varied from $x = 0$ to $x = 100$ mol.% in the initial charge) were prepared by solid-state reaction approach from ZnO and MgO powders (99.99% purity, with the grains of micrometer sizes) taken in required ratio to prepare the charge. The latter was pressed into pellets under the pressure 25 MPa and submitted to the sintering at $T = 1100$ °C for 3 hours in air and cooled down to room temperature with the furnace.

The X-ray diffraction (XRD) and IR reflection spectroscopy, as well as measuring of direct current conductivity were used for the sample characterization. For DC measurements, ohmic indium contacts were deposited onto the cleft sample surface, and the current-voltage characteristics were measured.

XRD patterns were registered in Bragg-Brentano geometry (θ–2θ) using a Philips X'Pert-MRD diffractometer with $\mathrm{Cu}_{K\alpha 1}$ radiation. Infrared reflection spectra were recorded using IRTracer-100 Fourier Transform Infrared Spectrophotometer equipped with a DRS-8000A diffuse reflectance tool. Excitation light angle of incidence was 13°. A gold mirror was used as a reference. The spectra were recorded with a resolution of 1 cm^{-1}. To reduce the roughness of the ceramic surface, its mechanical polishing was used.

3. Experimental results

3.1. X-ray diffraction

XRD patterns of samples with different MgO content in the charge show the reflexes from both hexagonal and cubic phases (Fig. 1). As can be seen, the position of $(002)_h$ peak of the hexagonal phase shifts toward larger angles with increasing the magnesium content, while $(100)_h$ peak shifts slightly toward smaller angles (for $x \leq 40$ mol.%) and then returns to larger angles as compared to the corresponding positions of the ZnO counterparts (Fig. 2). This corresponds to a decrease in the lattice parameter along the *c*-axis and, less pronounced, along the *a*-axis, which is indicative of Mg incorporation into ZnO lattice and formation of solid solution with hexagonal structure [11–14]. At the same time, the peak $(200)_c$ of the cubic phase shifts noticeably toward smaller

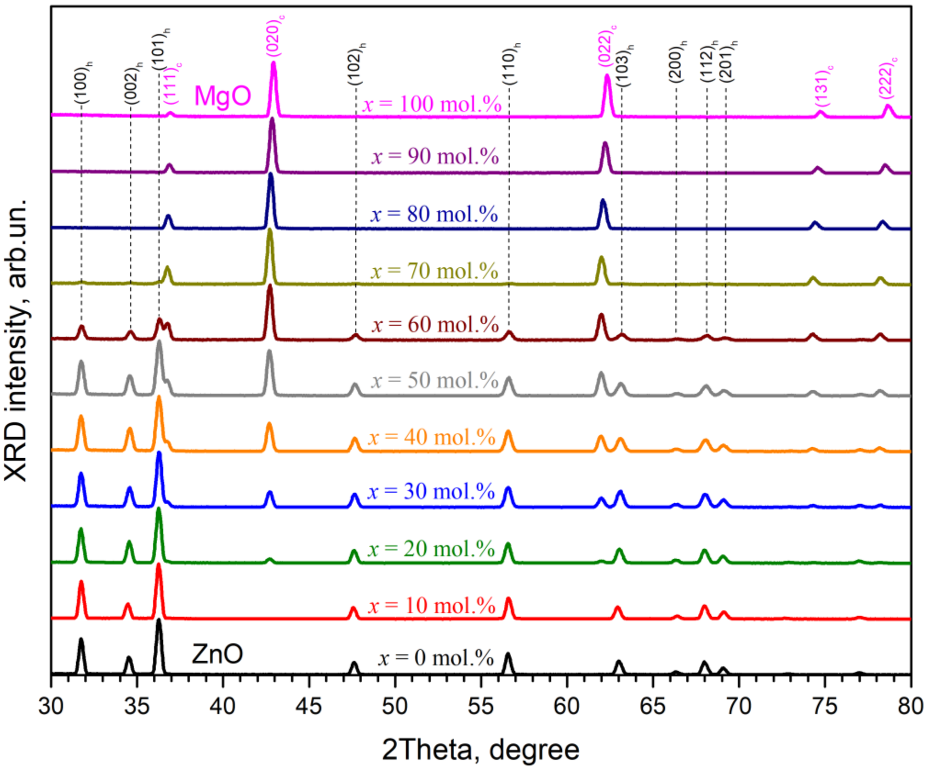

Fig. 1. XRD patterns of MgZnO ceramics with different MgO content in charge indicated in figure. The curves are shifted vertically for clarity.

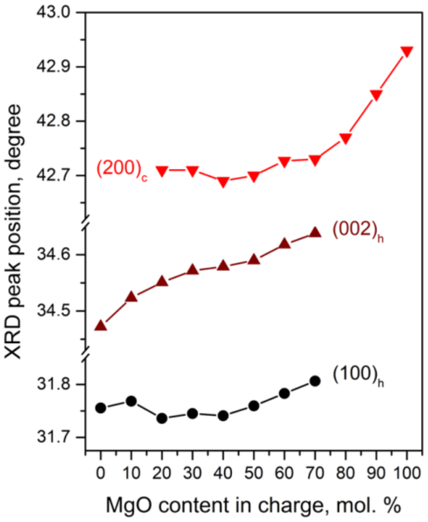

Fig. 2. Variation of $(100)_h$ and $(002)_h$ peak positions for the hexagonal phase and $(200)_c$ peak position for the cubic phases with MgO content in the charge.

angles when contribution of MgO (ZnO) decreases (increases) indicating Zn incorporation in MgO lattice and formation of solid solution with the cubic structure (Fig. 2). The increase of magnesium content results in the increase of cubic phase contribution as shown by the enhancement of (200) peak (Fig. 1). Fig. 2 shows that increasing the MgO content up to 70 mol.% leads to a monotonic shift of (002) peak position of hexagonal phase. It means that the sintering conditions used in this study did not allow achieving the solubility limit of Mg in ZnO even for the samples with the high MgO content in the charge (up to 70 mol.%). At the same time, the cubic phase peak shifts significantly when ZnO content increased up to 30 mol.% in the charge, and then this shift slows down, which may mean approaching the solubility limit of zinc in MgO that has been reported to be about 40 mol.% [13].

3.2. Direct current characterization

The dependences of DC conductivity of ceramic samples on the MgO content are shown in Fig. 3. As can be seen, addition of MgO reduces the DC conductivity. However, in the range of $x = 20…60$ mol.% the value of conductivity is weakly dependent on the MgO content, while at $x \geq 70$ mol.% the conductivity decreases sharply. Simultaneously, superlinearity of current-voltage characteristics increases, which can be explained by the influence of barriers on the value of DC conductivity. Therefore, to obtain information on the effect of magnesium content on the electrical characteristics of solid solution grains, the IR reflection spectra of the same samples were recorded and analyzed.

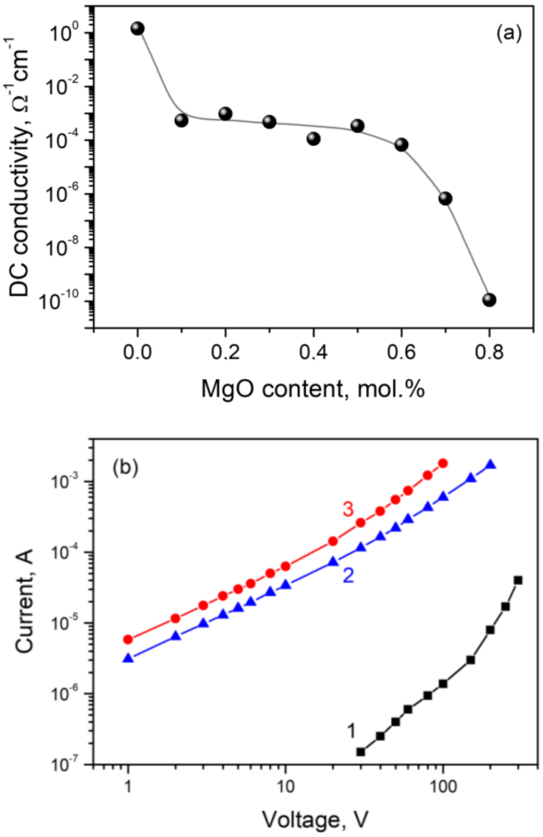

Fig. 3. Effect of MgO content in charge on the DC conductivity (a) and current-voltage characteristics of sintered ceramics (b). The MgO content was $x = 70$ (*1*), 60 (*2*), and 40 mol.% (*3*). $T = 300$ K.

3.3. IR reflection spectra

This study was performed for ZnO and solid solution ceramics with the MgO content $x = 10\ldots90$ mol.%. To simplify the presentation of these results, only more important experimental and simulated spectra will be displayed. Fig. 4 shows the $R(\nu)$ spectra for ZnO and (Mg,Zn)O solid solutions with $x = 20$, 60 and 80 mol.%.

To simulate IR reflection spectra, the interaction of infrared radiation with the phonon and plasma subsystems was considered. Theoretical calculation of the $R(\nu)$ spectra was performed within the range 200 up to 1100 cm^{-1} by using the approaches described in [15, 16]. The frequency dependence of dielectric constant as a function with additive and phenomenological contribution of phonon and plasma subsystems was considered. The multi-oscillator mathematical model with additive and phenomenological contribution of the oscillators of phonon subsystem into the dielectric constant was used.

The dielectric function was assumed to be complex, when the anharmonic interaction of the phonon and plasmon subsystems is taken into account in the imaginary form. To obtain information on the electrical and optical characteristics of crystallites from the IR reflection spectra, the method of dispersion analysis was used [17].

The frequency dependence of the dielectric function in the range of interaction of the phonon and plasmon subsystems was described by the expression for $\varepsilon(\nu)$ with account of the dumping coefficients for transverse and longitudinal optical phonons [18]:

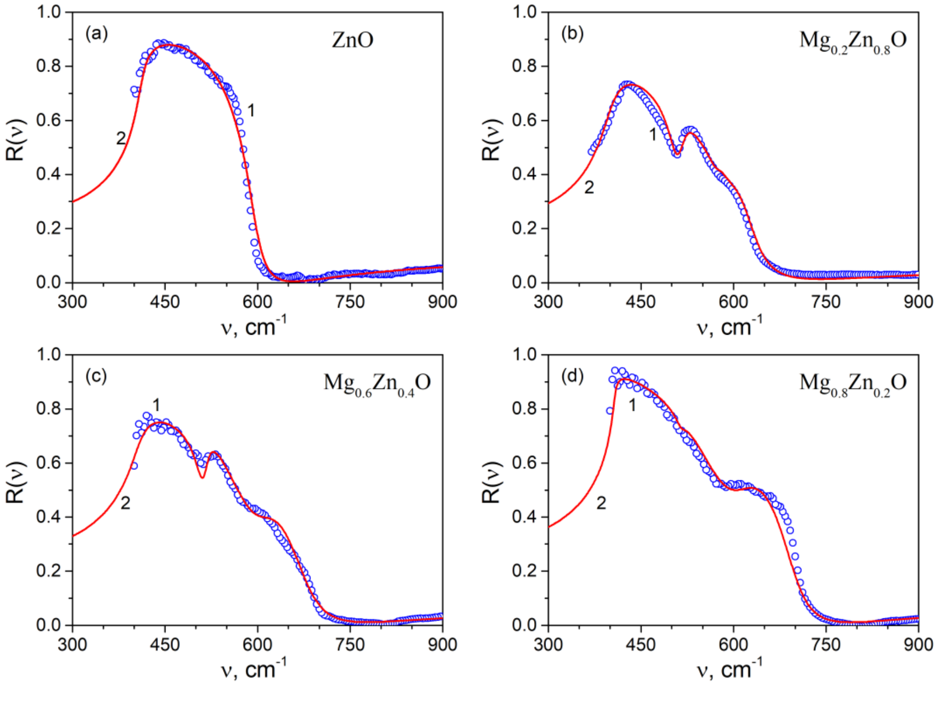

Fig. 4. Experimental (*1*) and simulated (*2*) IR reflection spectra $R(\nu)$ for ZnO (a) and (Mg,Zn)O (b, c, d) samples prepared with different MgO content in charge: 20 (b), 60 (c) and 80 mol.% (d).

Table. Electrophysical parameters of (Mg,Zn)O ceramics annealed at 1100 °C for 3 h *versus* MgO content in charge.

Sample composition		ν_p, cm^{-1}	γ_p, cm^{-1}	Concentration n_0, cm^{-3}	Conductivity σ, Ohm^{-1}·cm^{-1}	Mobility μ, cm^2/(V·s)
ZnO content in charge, mol.%	MgO content in charge, mol.%					
100	0	270	800	$8.40\cdot10^{17}$	3.75	27.9
90	10	350	640	$1.80\cdot10^{18}$	6.55	22.7
80	20	320	610	$1.50\cdot10^{18}$	5.72	23.8
70	30	280	680	$1.15\cdot10^{18}$	3.94	21.4
60	40	160	550	$3.8\cdot10^{17}$	1.61	26.5
50	50	120	400	$2.1\cdot10^{17}$	1.23	36.4
40	60	80	280	$9.4\cdot10^{16}$	0.78	51.9
30	70	50	110	$3.7\cdot10^{16}$	0.77	130.0

$$\varepsilon(\nu) = \varepsilon_{1j}(\nu) + i\varepsilon_{2j}(\nu) = \varepsilon_\infty + \varepsilon_{pj}(\nu) = \\ = \varepsilon_\infty \prod_j \frac{\nu_{LO,j}^2 - \nu^2 + i\gamma_{LO,j}\nu}{\nu_{TO,j}^2 - \nu^2 + i\gamma_{TO,j}\nu} - \frac{\nu_p^2\,\varepsilon_\infty}{\nu\left(\nu + i\gamma_p\right)},$$

where ν_{LO}, ν_{TO} are the frequencies of transverse and longitudinal optical phonons; γ_{TO}, γ_{LO} – attenuation coefficients for transverse and longitudinal optical phonons, respectively; γ_p and ν_p are the dumping coefficient and the plasma resonance frequency.

Simulation of the IR reflection spectra of the (Mg,Zn)O ceramics was performed with account of the contribution inherent to the hexagonal and cubic phases. As basic parameters of the (Mg,Zn)O phonon subsystem, the values obtained by the authors [19] were used, and they were then varied when modeling the experimental spectra.

Using the Lyddane–Sachs–Teller relation and the method of dispersion analysis of the IR reflection spectra in the high-frequency range, the value of high-frequency dielectric function was evaluated to be $\varepsilon_\infty = 3.28$. As can be seen from Fig. 4, the theoretical results are in good agreement with the experimental data. A similar agreement was obtained for the other values of x.

It follows from Fig. 4 that $R(\nu)$ spectra of the samples with x = 20…60 mol.% in the range of 507…511 cm^{-1} show a minimum that corresponds to the LO-phonon of the hexagonal phase of the solid solution [20]. Thus, in the samples with $x < 60$ mol.%, this phase makes a main contribution to IR reflection spectra. However, in the case of larger x-values the modeling of IR spectra also requires accounting the contribution of phonons in this phase. It means that in the samples with this x the hexagonal phase is also present, despite the reduction in its contribution. In the case of x increasing from 70 up to 80 mol.%, within the range 580…640 cm^{-1} a plateau was recorded experimentally and modeled, where $R(\nu) = 0.5$, which is associated with the transverse optical phonon of the cubic phase solid solution.

As the calculation shows, the plasmon subsystem makes a contribution to the IR reflection spectra in (Mg,Zn)O ceramics with $x \le 70$ mol.%, which allowed determination of the values of concentration, conductivity and electron mobility in solid solutions. At $x > 70$ mol.% the contribution of plasmon to the IR reflection spectra is not registered.

As shown in Table, in solid solution ceramics with $x \le 30$ mol.%, the concentration of free electrons in the grains practically does not differ from its value in ZnO. As the contribution of magnesium oxide increases, the electron concentration decreases. Simultaneously, a significant increase of the contribution of cubic phase solid solution is observed in XRD patterns.

4. Discussion

As it was mentioned above, addition of MgO reduces the DC conductivity as compared to that of ZnO ceramics. However, within the range x = 20…60 mol.% the value of conductivity is weakly dependent on the MgO content, while at $x \ge 70$ mol.% the conductivity decreases sharply, and superlinearity of the current voltage characteristics increases. At the same time, for all the solid solution samples where plasmon was registered the DC conductivity value remains much smaller than the value obtained from simulation of IR reflection spectra. It indicates the presence of barriers in the ceramic at all this x values. However, the nature of barriers may depend on the magnesium content. As it was shown in [18], at small x, when the hexagonal phase is dominant, the DC conductivity is defined by the conductivity of densely sintered grains of the hexagonal phase of the solid solution. In this case, the barriers may be caused by the slightly different Mg content in the grains of the hexagonal phase, which can lead to variations in the band gap of solid solution. At the same time, at $x \ge 70$ mol.% due to the increase in the number of grains of the cubic phase, the barriers may be related with the boundaries between the grains of the hexagonal and cubic phases of

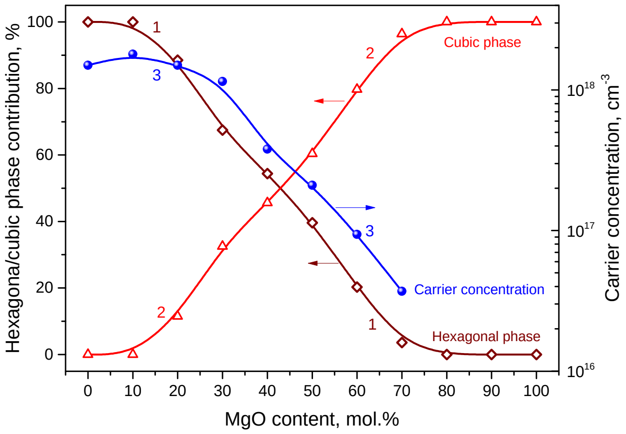

Fig. 5. Dependences of hexagonal (*1*) and cubic (*2*) phases contribution as well as the concentration of free electrons (*3*) on the MgO content.

the solid solution. It is consistent with the increase in the superlinearity of the current-voltage characteristics, which indicates increasing barrier contribution in the conductivity as compared to the samples with a smaller x.

For a more detailed analysis of the plasmon origin and the reasons of electron concentration decrease, we compared the dependence of contribution inherent to the hexagonal and cubic phases on x with the corresponding dependence of the electron concentration. The contribution of the hexagonal and cubic phases to the ceramic samples was estimated from the ratio of the intensity of the XRD peaks from the hexagonal (101) and cubic (200) phases of the solid solution taking into account the masses of zinc and magnesium. The dependence of the contribution of these phases on x is presented in Fig. 5. As can be seen from the figure, the contribution of the hexagonal phase decreases with increasing x, and at $x \geq 80$ mol.% it is not observed in the XRD patterns. Fig. 5 also shows that this phase up to $x < 40$ mol.% is dominant. At the same time, at $x > 60$ mol.% the contribution of cubic phase in ceramics significantly exceeds the contribution of hexagonal one. It may cause the influence of barriers between these two phases on the value of DC conductivity at $x > 60$ mol.% and result in the sharp increase in the superlinearity of current-voltage characteristics.

Fig. 5 also shows that the increase of MgO content up to 30 mol.% does not significantly change the concentration of free electrons and this concentration is close to the value observed in ZnO ceramics ($x = 0$). Since at $x \leq 30$ mol.% the hexagonal phase is dominant, it can be concluded that the plasmon registered in the IR reflection spectra, as well as the electron concentration determined from it belong to this phase of the solid solution. At the same time, this concentration is unlikely for the cubic phase (even if the solubility limit of zinc in MgO is 40 mol.%). Since the value of ZnO conductivity is determined by interstitial zinc (Zn_i) [20], it can be supposed that in the hexagonal phase of the solid solution this defect also is the main donor.

With increasing the MgO content in charge to $x \geq 40$ mol.%, the concentration of carriers begins to decrease, and for $x = 70$ mol.% it is $n = 3.7 \cdot 10^{16}$ cm^{-3}, while for higher x values plasmon is not observed. Since in the latter case the cubic phase of the solid solution is dominant, it can be concluded that this phase, at least with low zinc content, is high-resistive.

As can be seen from Fig. 5, the decrease in the electron concentration correlates with the decrease of the hexagonal phase contribution in ceramics. Therefore, we can assume that in all cases, plasmon is a characteristic of this phase. In this case, the decrease of n_0 with increasing x may be caused, for example, by a decrease in the concentration of interstitial zinc due to the increased energy of its formation [2, 3]. Another reason may be a decrease of Zn_i concentration in the hexagonal phase due to zinc extraction to form a cubic phase. At the same time, a similar dependence of the electron concentration on x can be expected for the cubic phase of the solid solution, which at low x (*i.e.*, a high zinc content) can have a significant conductivity, which decreases with increasing x due to a decrease in the zinc content. However, as noted above, the large value of n_0, which is observed at small x, *i.e.*, at the maximum possible zinc content in MgO, coincides with n_0 in ZnO, which is unlikely for the cubic phase.

Since the solubility limit of Mg in ZnO does not exceed 20 mol.% [21], and the cubic phase, at least at large x, is high-resistive, it is logical to assume that the decrease in electron concentration for the samples with a high MgO content (x = 40…70 mol.%) is due to a decrease in the Zn_i content in the hexagonal phase of solid solution exactly because of zinc extraction to form the cubic phase.

5. Conclusion

The structural and electrical characteristics of (Mg,Zn)O ceramics with a different magnesium content were studied using XRD diffraction, specular IR reflection as well as direct current methods. Being based on the analysis of IR reflection spectra and their comparison with the contribution of different phases to ceramic sample, it has been shown that the conductivity of the grains of hexagonal phase is much higher than the conductivity of the cubic structure grains. The electron concentration in the grains of hexagonal phase up to $x = 30$ mol.% is close to its concentration in ZnO ceramics. It has been supposed that the conductivity of hexagonal phase of solid solution is defined by interstitial zinc that is the main donor in this phase. The decrease of the electron concentration with the decrease of this phase content in ceramic sample has been observed and explained by the decrease in the interstitial zinc content due to zinc extraction to form the cubic phase. The DC current measurements have shown the lower conductivity as compared to the value estimated from the IR reflection spectra. This fact as well as the superlinearity of current-voltage characteristics has shown the influence of spectra. This fact as well as the superlinearity of current-voltage characteristics has shown the influence of barriers on the DC conductivity, which does not allow obtaining information on the concentration of free electrons in the grain. It has been concluded that at low x the barriers are obviously caused by inhomogeneous doping of different ZnO grains, while at $x \geq 70$ mol.% they may be related with the boundaries between the grains of the hexagonal and cubic phases of the solid solution.

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Залежність електричної провідності кераміки $Mg_xZn_{1–x}O$ від фазового складу

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Анотація. Твердофазною реакцією при 1100 °С протягом 3 годин одержано кераміку (Mg,Zn)O з різним вмістом MgO, що змінювався у межах від 0 до 100 мол.% у шихті. Досліджено структурні та електричні характеристики кераміки методами рентгенівської дифракції та спектроскопії інфрачервоного відбиття, а також за допомогою прямого вимірювання електропровідності методом постійного струму. Показано, що величина електропровідності, визначена при моделюванні внеску плазмону у спектри інфрачервоного відбиття, характерна для гексагональної фази твердого розчину, оскільки у кубічній фазі твердого розчину плазмон не проявляється. Встановлено, що концентрація електронів у зернах гексагональної фази (Mg,Zn)O у зразках, виготовлених із шихти із вмістом MgO до 30 мол.%, близька до концентрації носіїв у кераміці ZnO. При збільшенні вмісту MgO спостерігається зменшення внеску гексагональної фази у керамічних зразках, що супроводжується зменшенням концентрації електронів і пояснюється зменшенням вмісту міжвузлового цинку внаслідок його екстракції з ZnO для утворення кубічної фази твердого розчину. Прямі вимірювання електропровідності при постійному струмі показують менші значення провідності у порівнянні із значеннями, оціненими зі спектрів інфрачервоного відбиття. Цей факт, а також надлінійність вольт-амперних характеристик можна пояснити наявністю міжзерених бар'єрів, що перешкоджають визначенню концентрації вільних електронів у зернах. Природа цих бар'єрів, а також роль міжзеренних границь у провідності зразків на постійному струмі, обговорюються.

Ключові слова: кераміка MgZnO, дифракція рентгенівських променів, електрична провідність, спектри ІЧ-відбиття.