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Comparative analysis of the effectiveness of transparent conductive coatings based on various materials

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Abstract. Transparent conductive oxide materials, which are used mainly as transparent electrodes, but have also found applications in optics, photonics and instrumentation. The main material used in production is indium oxide, alloyed with tin. However, indium is a rather expensive material, as well as a rare one. In this regard, the analysis of alternative materials made of transparent conductive oxide is relevant. Transparent conductive oxide materials are mainly used as transparent electrodes, but have also found applications in optics, photonics and instrumentation. The main material used in production is indium oxide fused with tin. However, indium is a rather expensive material, as well as a rare one. In this regard, the analysis of alternative materials made of transparent conductive oxide is relevant. The materials under consideration are gallium oxide doped with indium and antimony, tin oxide doped with fluorine and antimony, zinc oxide doped with gallium and aluminum. The analysis of the main parameters of transparent conductive oxides is carried out, a method for evaluating the effectiveness of materials according to technical and economic criteria is proposed. The methodology is based on the Laplace criterion, the compilation of a matrix of the effectiveness of materials. According to the proposed methodology, taking into account the target effect and the cost of obtaining the studied films, the effectiveness of promising transparent conductive materials was evaluated.

Keywords: transparent conductive oxide, indium oxide, zinc oxide, tin oxide, effectiveness

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Сравнительный анализ эффективности прозрачных токопроводящих покрытий на основе различных материалов

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Аннотация. Прозрачные проводящие оксиды – материалы, которые в основном используются в качестве прозрачного электрода, но также нашли применение в оптике, фотонике и приборостроении. В качестве материалов рассмотрены оксид индия, легированный оловом, оксид олова, легированный фтором и сурьмой, оксид цинка, легированный алюминием и галлием, оксид галлия, легированный индием и сурьмой. Предложена методика обоснованного выбора оптимального прозрачного проводящего оксида как по наибольшей технологической эффективности, так и по технико-экономической эффективности с учетом технологических параметров и затрат на получение тонкопленочного покрытия.

Ключевые слова: прозрачные проводящие оксиды, оксид индия, оксид олова, оксид цинка, эффективность

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Introduction

One of the promising and actively developing areas of electronics is thin-film electronics. Thin films have found application in many sectors of the semiconductor and optoelectronics industries [1, 2]. The segment of thin-film structures in the form of transparent conductive oxides requires special attention. The most common transparent conductive oxide (TCO) films are SnO_2, In_2O_3, GaO and ZnO [3–5]. At the present stage of technology development, indium tin oxide can be attributed to materials with the best functional properties. However, its high cost and scarcity indicate the relevance of choosing an alternative material for TCO [6, 7]. An important task is to achieve values of the transmittance of thin films in the visible range of the spectrum of more than 85%, resistivity – no more than 10^{-4} Ohm·cm.

Materials and Methods

The materials being compared are transparent conductive oxides, for which the main performance targets are coating resistance and throughput; other parameters indirectly affect these properties.

Properties were studied on coatings of the same thickness (250 nm ± 10 nm). The table shows a comparison of transparent conductive oxides according to the specified parameters.

Table 1

Comparison of materials used as transparent conductive oxides in terms of transparency and conductivity

Header	Samples of transparent conducting oxides						
	In_2O_3:Sn	SnO_2:F	SnO_2:Sb	ZnO:Ga	ZnO:Al	GaO:In	GaO:Sb
R (surface resistance), Ohm·cm	2.4×10^{-4}	5×10^{-4}	10^{-3}	10^{-3}	10^{-2}	2×10^{-3}	4×10^{-3}
D (transmittance), %	95	83	92	85	90	90	88

In addition, calculations of parameters such as concentration, mobility of charge carriers, and band gap were performed.

Table 2

Estimation of the band gap width, concentration and mobility of charge carriers

	In_2O_3:Sn	SnO_2:F	SnO_2:Sb	ZnO:Ga	ZnO:Al	GaO:In	GaO:Sb
Eg (band gap width), eV	4	4.41	3.75	3.59	3.52	–	–
n (concentration of charge carrier), cm^{-3}	1×10^{20}	4.6×10^{20}	2×10^{20}	10×10^{20}	4.7×10^{20}	4×10^{20}	3×10^{20}
μ (mobility of charge carriers) $cm^2/(s\times V)$	12	28	10	10	14.7	10	10

Based on the studies performed, it is advisable to conclude that the following are the optimal materials according to the criterion of the highest electrical conductivity: In_2O_3:SnO_2 and SnO_2:F. At the same time, from the point of view of optical application, In2O3:SnO2, SnO2:F and SnO_2:Sb can be singled out as priority materials. Based on the analysis, tin is a promising and currently undervalued material. In order to make a reasonable choice of a transparent conductive oxide, a matrix of the effectiveness of transparent conductive oxides has been compiled. The use of materials as a transparent conductive oxide dictates the need to ensure high transparency and conductivity, therefore, In_2O_3 materials: SnO_2 and SnO_2:Sb have found the greatest use to date, which is confirmed by the experimental data presented in the Tables 1, 2.

In order to determine the optimal material based on a set of significant technological parameters and cost factor, the authors propose a method for the reasonable selection of the optimal transparent conductive oxide both for the highest technological efficiency (excluding the cost factor for the technological process) and for technical and economic efficiency (taking into account technological parameters and costs). The methodology is based on the use of the Laplace criterion used in system analysis to select the optimal alternative. As essential technological parameters (by which technological efficiency is evaluated) the surface resistance and transmission coefficient are considered.

Initial data: alternative materials are available for the production of transparent conductive oxides. The indicators of surface resistance and transmittance, characterizing the target effect of using a transparent conductive oxide are known. The task is to choose the optimal material, which has the highest efficiency.

Results and Discussion

The compiled efficiency matrix is presented in Table 3, which also contains the values of the corresponding cost indicators. The dimensionless value of g_l is the cost ratio of obtaining a transparent conductive oxide to the maximum allowable costs; R_{il} is the ratio of the surface resistance to the maximum permissible (the maximum permissible surface resistance is 10^{-2} Ohm·cm), D_{il} is the ratio of the transmission coefficient to the maximum permissible.

Next, the efficiency of transparent conductive oxides is calculated and the efficiency of materials is compared based on the method based on the Laplace criterion.

For each materialal, it is necessary to calculate the efficiency $K(a_l)$ according to technological parameters (surface resistance and transmission coefficient) using the formula:

$$K(a_l) = p_1 \cdot \frac{1}{R_{il}} + p_2 \cdot \frac{1}{D_{il}}, \quad (1)$$

where p_1, p_2 is the coefficient that takes into account the priority of parameters $\frac{1}{R_{il}}$ or $\frac{1}{D_{il}}$ of the material.

The values of p_1, p_2 are determined by expert assessments. In the case under consideration, equal priority is given to the importance of the required values of surface resistance and transmission coefficient, that is, $p_1 = p_2 = 0.5$.

Table 3

Efficiency and cost matrix for materials used in software

Material	Material designation, a_1	$\frac{1}{R_{il}}$	$\frac{1}{D_{il}}$	g_1
$In_2O_3:SnO_2$	a_1	$\frac{1}{2.4\cdot10^{-2}}$	$\frac{1}{1.19}$	0.68
$SnO_2:F$	a_2	$\frac{1}{5\cdot10^{-2}}$	$\frac{1}{1.04}$	0.48
$SnO_2:Sb$	a_3	$\frac{1}{10^{-1}}$	$\frac{1}{1.15}$	0.43
ZnO:Ga	a_4	$\frac{1}{10^{-1}}$	$\frac{1}{1.06}$	0.45
ZnO:Al	a_5	1	$\frac{1}{1.125}$	0.49
GaO:In	a_6	$\frac{1}{2\cdot10^{-1}}$	$\frac{1}{1.125}$	0.59
GaO:Sb	a_7	$\frac{1}{4\cdot10^{-1}}$	$\frac{1}{1.1}$	0.49

Then $K_1 = 0.5\left(\frac{1}{2,4\cdot10^{-2}}+\frac{1}{1.19}\right)=22.42$, similarly, K_2 = 10.48; K_3 = 5.43; K_4 = 5.47; K_5 = 0.94; K_6 = 2.94; K_7 = 1.7.

Then the optimal technological efficiency K_{opt} is determined as the largest value of seven values of $K(a_l)$. In the case under consideration K_{opt} = 22.42, therefore, according to the technological parameters (for the target effect), the optimal material, designated a1, $In_2O_3:SnO_2$ is taken.

To account the impact of the cost factor, the aggregating function $K(a_l, g_l)$ is defined as the ratio of efficiency $K(a_l)$ to the cost factor g_l:

$$K\left(a_l, g_l\right) = \frac{K\left(a_l\right)}{g_l}. \tag{2}$$

In the case under consideration, $K\left(a_1,\ g_1\right) = \frac{22.42}{0.68} = 32.97$, similarly, $K(a_2, g_2)$ = 21.83; $K(a_3, g_3)$ = 12.6; $K(a_4, g_4)$ = 12.15; $K(a_5, g_5)$ = 1.92; $K(a_6, g_6)$ = 4.58; $K(a_7, g_7)$ = 3.46.

Next, the optimal material is determined according to the target effect and cost factor $K(a_l, g_l)$, having:

$$K\left(a_l, g_l\right)_{opt} = max\left(l\right)\frac{K\left(a_l\right)}{g_l}. \tag{3}$$

In this case $K(a_l, g_l)_{opt}$ = 32.97, therefore, according to technical and economic indicators, the optimal material is $In_2O_3:SnO_2$.

Conclusion

A methodology is proposed for the reasonable selection of the optimal transparent conductive oxide both in terms of technological parameters and taking into account the cost of obtaining materials. The methodology is based on the Laplace criterion, takes into account the priority of the importance of the parameters of materials (priority is determined by expert assessment and depends on the specific field of application of the material), depending on which efficiency is calculated according to technological parameters. In the case when, in addition to technological parameters, the cost of obtaining materials is decisive, then efficiency is calculated according to technical and economic parameters in the form of an aggregating function. The proposed technique has been tested to identify transparent conductive oxides with optimal technological parameters (surface resistance, transmission coefficient) and the lowest cost of obtaining them.

The result of the research is the identification of the most suitable materials for use in TCO, which are In_2O_3:SnO_2 and SnO_2:F. In this case, from the point of view of optical application, the priority materials can be In_2O_3:SnO_2, SnO_2:F and SnO_2:Sb. Based on the analysis, tin is a promising and undervalued material. The materials use as a transparent conductive oxide requires high levels of both transparency and conductivity, therefore the materials In_2O_3:SnO_2 and SnO_2:Sb have found the greatest application today, which is confirmed by the experimental data presented in the tables. Taking into account technical and economic indicators, the optimal material is In_2O_3:SnO_2.

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