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Simulation of the Mechanism of Defect Structure Formation in Polycrystalline Indium Oxide Under Ion Irradiation »

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The structural changes in polycrystalline indium oxide were studied before and after irradiation of samples, Xe^+ ions with energy 140 and 300 keV, X-ray methods. Discovery, that irradiation leads to a change in the chemical composition of the oxide, accompanied by phase transformations. The main structure of the cubic oxide after irradiation contain macro and micro stresses, which depend on the energy irradiation. The increase in the relative integral intensity of radiation reflected from the planes of the cell on depth was observed. The maximum value observed at a depth of 1.5 μm from the plane (510). The analyses of reflected the radiation found that the flux of photons remains constant - the atomic nuclei of oxide not change, increases the frequency, decreases the wavelength depend from the energy irradiation. In some directions in reflecting from the planes, the atoms are formed with different electron density, that connect whit presence of defects, which leads to appear of the forced oscillation, which increases the relative integral intensity of the reflected radiation. These processes are damped with increasing depth of the sample.

Keywords: Indium oxide, Structural defects, Phase transitions, Stresses.

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1. INTRODUCTION

Indium oxide has a high melting point. It is a semiconductor-n-type, has a structure of type C and contains 25 % naturally ordered anion vacancies, which are elements of the structure. Such defects can be combined with the atoms impurity at the different effects on the material and form the complexes defects. The accumulation of such defects changes the structure and properties of the semiconducting oxide materials.

Materials from the In_2O_3 are of practical interest as materials with electrical conductivity, which can be used in various fields of engineering and agriculture: in the form of solar energy converters, as sources of energy, solid fuels, materials of electronics [1-3].

Changes in the physical properties of polycrystalline indium oxide at thermal treatment were investigated in [4, 5]. It is interesting to investigate the effect of ion irradiation on the material of the layers oxide of indium, which deep from implant layer. Since this material can be used in converters of energy.

The purpose of this work is to model the mechanisms of defect formation in a polycrystalline indium oxide after irradiation by Xe^+ with energy at 300 keV and their influence on the structural properties.

2. RESEARCH RESULTS

2.1 Materials and methods research

Samples were prepared from powders of In_2O_3 brand os.ch. sintered in the temperature range 1000 – 1600 °C in air, followed by quenching in air and under oxidation 1200 °C in the air to constant weight. Mass loss with an accuracy of ± 0, 0002, the samples were of $InO_{1,5}$ with the following properties: unit cell parameter a = 1.0120 nm, density of 7.110 g/cm^3 is the X-ray, density of hydrostatic – 6.282 g/cm^3, harden –7900 H/mm^2

Phase composition and lattice parameters were determined by X-ray. The lattice parameter was determined with an accuracy of ± 0.0001 nm, use method of building the profile of X-ray lines from points in the angular range 10-700 of 2θ.

Samples before irradiation and after mounted in a holder with a fixed position, which allowed, after all the operations to explore the same position of patterns in the radiation of monochromatic Cu K -α with a wavelength of 0.1540 nm.

Irradiation was performed at 25°C in a system with a cryogenic shroud, located at the temperature liquid nitrogen, dose 2×10^{16} cm^{-2} at energies of 140 and 300 keV.

Table 1 – Parameters of the implanted oxide layer during ion irradiation dose of Xe^+ , $2 \cdot 10^{16}$ cm – 2

The energy of irradiation	140 keV	300 keV
Limiting the dose of implantation, cm^{-2}	$2{,}7\cdot10^{16}$	$4{,}9\cdot10^{16}$
The average concentration of implanted impurity, cm^{-3}	$4{,}6\cdot10^{21}$	$3{,}6\cdot10^{21}$
The average energy transferred to the atom, eV	166	182
The thickness of the implanted layer, cm	$1{,}1\cdot10^{-5}$	$2\cdot10^{-5}$
The thickness of the sprayed layer, cm	$4{,}1\cdot10^{-6}$	$4{,}1\cdot10^{-6}$
The life time of the peak, s	$9{,}5\cdot10^{-10}$	$9{,}3\cdot10^{-9}$
The pressure in the zone of peak, Pa	$1{,}5\cdot10^{-13}$	$1{,}1\cdot10^{-13}$
The pulse peak power in the area, Ns	$7{,}4\cdot10^{-13}$	$1{,}2\cdot10^{-11}$

The depth of the investigated layer was determined by taking into account the absorption and scattering coefficients for X-rays of indium oxide according to [6, 7]. The thickness of the investigated layer on the angle of diffraction is shown in Figure 1. The dependence is linear. This approach allows us to study the properties of oxide depth.

The stresses in the oxide of indium after irradiation the samples were determined harmonic analysis, the modulus of elasticity E and coefficient of Poisson is taken from the data of [8, 9].

2.2 A mathematical model of recovery of indium oxide under ion irradiation

After irradiation of the samples ions Xe^+ with energies of 140 and 300 keV are changed: the color samples from yellow to black to a depth of 2×10^{-3} m, changing the phase composition. On the X-ray photograph appear weak lines of monoclinic, hexagonal form of indium oxide, which were previously observed during heat treatment in vacuum, and the present line of metallic indium, the line intensity increases with the irradiation energy. These facts are indicate on the formation in the structural defects of the oxygen, that lead to the appearance of centers color in the samples, the complete restoration of the surface layer of oxide samples.

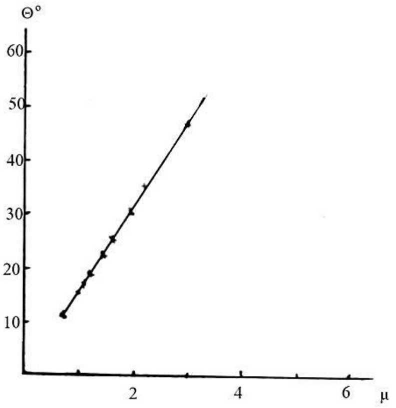

Fig. 1 – The dependence of the diffraction angle on the depth of the sample In_2O_3, μ- μm

Recovery of indium oxide at irradiation lead to form: the color centers, the presence of oxygen-depleted phases and carried out by the following model (1)

$$In_2O_3 \rightarrow In_{2-y}O_{3-x}\upsilon[F]_x + In_y^{3+} + \frac{x}{4O_2}\uparrow \qquad (1)$$

where x – deviation from the order in of oxygen, the y – the proportion of metallic indium, $\upsilon[F]$ – color centers, which are formed by reaction (2)

$$In^{2+} + \upsilon(O) \rightarrow In^{3+} + \upsilon[F] \qquad (2)$$

The change in free energy associated with the restoration of the oxide is determined by the following relationship (3)

$$\Delta\Phi = \left(\frac{\phi_{\upsilon(O)}}{2} - \frac{\phi_{\upsilon[F]}}{2} + A - \frac{F}{4}\right)x + \phi(y) - T\Delta S \qquad (3)$$

where $\phi_{\upsilon(O)}$ – anion vacancy formation energy, $\phi_{\upsilon[F]}$ – energy of formation of color center, A – energy electron affined of the anion, F – transition energy of oxygen in the gas phase, $\phi_{[In]}$ – the energy of formation of metallic indium.

Entropy in the process of recovery oxide is determined by (4)

$$T\Delta S = kT\ln x = \gamma kT \ln\frac{\Delta V}{V} \qquad (4)$$

where ΔV – the change in volume of the unit cell in the formation of additional anion vacancies as a result of irradiation by xenon, γ – a coefficient that takes into account the change in volume around the defect, as the ratio of the radius to the radius of the anion vacancies of oxygen.

In the study of the diffraction lines in the angular range 10-70° of 2θ, the interval of angles determines the depth of 0.7-2 μm sample before and after irradiation. The strong changes observed in the profile of the lines of: changing the intensity, position, width. For an example show on figure 2 the diffractions lines from planes (332) (510) (440), which characterize the change in the structure of indium oxide in the depth of the sample.

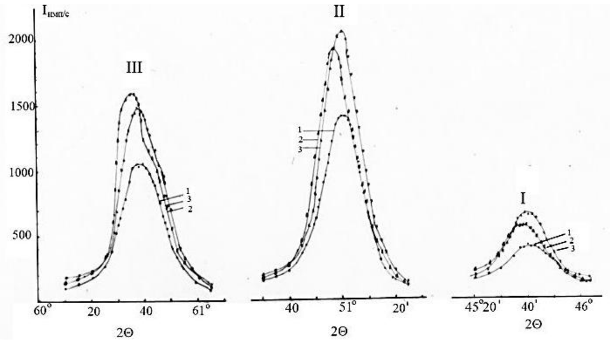

Fig. 2 – Profiles of X-ray reflections from the planes of 1 – (332) 11 – (510) 111 – (440) 1 - before irradiation, 2 – after irradiation by xenon ions with energies of 140 keV, 3 – after irradiation by xenon ions with an energy of 300keV

1. Macro stresses indium in the oxide (Fig. 3) after irradiation with xenon ions at energies of 140, 300 keV decreases from the surface of 0.7 - 1.2 mm, attenuate to a depth of 2 mm and practically coincide at this depth.
2. Changes in the relative integral intensity of X-ray lines of samples indium oxide after irradiation by xenon ions with energies of 140, 300 keV at a depth of 0.7-1.5 mm, virtually identical to the slopes of lines and vary in size depending on the energy irradiation. It should be noted that the relative integrated intensity of the reflections from the (510) increases with energy 140, 300 keV, and for reflections from planes (440) (622), which decrease corresponds to the depth of the sample (1.5-2) mm, the relative integral intensity almost the same for samples irradiated by xenon ions from values of energy.
3. Micro stresses of samples after irradiation energies of 140, 300 keV changes equally from the slope of a small difference on values. It should be noted that at a depth of 0.7-0.9 micron micros tresses decrease to negative values, and then increase with the same slope at a depth of 0.9-2 microns. These changes indicate the micros tress distribution of the wave nature of the micro stresses in the depth of the sample.

Availability: stresses in the samples after irradiation by xenon ions with different energies and the anomalous increase in the intensity of reflections from planes in depth, indicate the complexity of the effects of irradiation on the structure of indium oxide. This mechanism can be explained by assuming that with the relative probability of the growth of the integrated intensity of reflections from the planes of the unit cell is the depth of the stream of photons – CuK_α with a wavelength of 0.1540 nm.

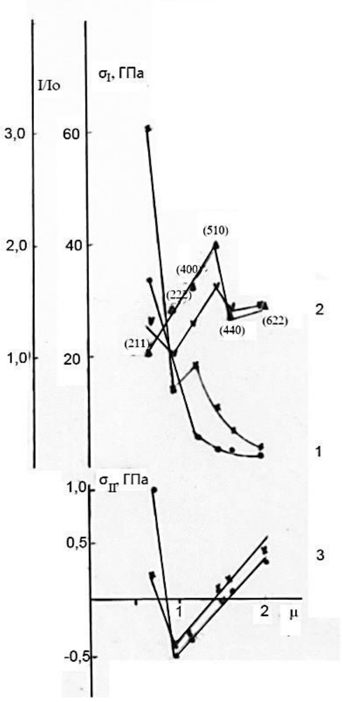

Fig. 3 – Distribution macro stresses: ● -140 keV x 300 keV and 2 - to change the relative integral intensity of X-ray lines: v – 140 keV; ▲ – 300 keV, 3 – micro stresses: ● -140 keV x-300 keV

Necessary to analyze the flow of photons reflected from the planes in depth, depending on the energy of xenon ions irradiated samples. Analyze the increase in the intensity of reflections from the (510) depending on the energy irradiated (Table 2).

The flow of the reflected photons can be estimated by the following equation (5)

$$N(x) = \frac{I(x)}{h\omega} \qquad (5)$$

where $N(x)$ is the photon flux at depth x μm (reflection from the respective planes); $I(x)$ is the intensity of the reflections, imp/s; h is Planck's constant; ω is the oscillation frequency [10].

The resulting estimates (Table 2) show that the reflected photon flux remains constant; this indicates that the nuclei of oxide are not destroyed. The reducing of the wavelength, growth frequency of the oscillation, increased energy reflected from the plane (510), indicate the photon flux induced oscillations of the photons. These streams of photons reflected from a depth of 1.5 microns. At this depth micro stresses change sign on the magnitude macro stresses depending on the energy of radiation are reduced. Forced oscillations of the reflected photons appears to be associated with the ordering of defects in the structure of indium oxide and the creation of lines in the plane containing atoms change in electron density.

Table 3 – Analysis results of reflections from the (510), depending on the irradiation energy for the ions Xe + dose $2 \cdot 10^{16}$cm^{-2}

The energy irradiated	standard	140 keV	300 keV
ω – The frequency of oscillation, 10^{17} Hz	19,48	28,47	35,96
The flux of photons, 10^{17} imp. c/J	10,07	10,07	10,07
λ – Wavelength, 10^{-9} m	0,1540	0,105	0,080
The energy of flow keV	8	11,77	14,8

The mechanism of formation of defects in the structure of indium oxide under ion irradiation is very different from the thermal and electrical effects on indium oxide [4,5].

CONCLUSIONS

At irradiation of samples of indium oxide of Xe$^+$ ions, take place a change in chemical composition, followed by a phase transformation, at a depth exceeding the thickness of the layer of doped ions. Structural changes in the depth of polycrystalline indium oxide are wavy in nature and depend strongly on the irradiation energy of ions xenon. The mechanism of formation of defects in the oxide structure differs significantly from the thermal effect on the indium oxide. The mathematical calculation of the intensity of reflecting radiation and determined that the atoms of indium oxide cores do not change, and the intensity of the reflections increases due to forced vibrations associated with different electron density of atoms in the reflecting planes.

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