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In this paper, the transformations of the morphology and surface structure of CdTe crystals under the action of pulsed laser irradiation and the properties of laseroptimized Schottky diode X/ $\gamma$ -ray detectors developed by Ni and NiO deposition onto commercially available (111) oriented CdTe:Cl wafers have been investigated. Using scanning electron and atomic force microscopy, it was shown that, depending on the energy density and laser pulse duration, the morphology, phase composition and distribution of the system of defects and inclusions in the surface areas of CdTe crystals can be optimized. A detailed analysis of the effects of laser treatment on the electrical and spectrometric properties the CdTe X/γ-ray detectors under study was also carried out.

### INTRODUCTION

For several decades cadmium telluride (CdTe) maintains its position as the major material for X/γ-ray detectors widely used in science, technology, security, medicine and other fields. However, the manufacturers of CdTe detectors have faced a variety of problems. One of them is the problem of preparation of metal-semiconductor structures with low leakage current, which is a source of electrical noise and decreases the energy resolution of the devices. In the late 1990s a number of publications by T. Takahashi et al. [1,2] reported on the results testifying to exceptionally high performance of CdTe detectors with Pt/p-CdTe/Pt contacts and In/p-CdTe/Pt Schottky barrier having no special scheme for electric signal processing in the detector circuit. Later we reported significant improvement in X/y-ray detector performance achieved by forming both rectifying and near-ohmic contacts by the deposition of Ni on the opposite surfaces of semi-insulating CdTe crystals [3].

In the present work, we continue the investigation of CdTe Schottky diode detectors produced by deposition of different contact materials onto pre-cleaned commercially available detector-grade (111) oriented CdTe wafers with an area of  $5 \times 5$  mm<sup>2</sup> and thickness of 0.5 mm [4-6]. Laser treatment of Schottky contacts using millisecond YAG-laser has been carried out in order to modify and improve their structure and phase state. The morphology, structure, and composition of thin layers before and after laser treatment were studied by atomic-force and scanning electron microscopy. The effects of laser treatment on the electrical properties of CdTe X- and γ-ray detectors under study were also studied. The combination of the open-circuit voltage decay and high-frequency impedance measurements allowed determination of the dominant recombination and transport mechanisms of charge carriers in the rectifying detector structures under different levels of excitation and temperatures. The deep understanding of these processes and their dependence on the type of employed rectifying junctions and contacts is critical for efficient charge-carrier collection within the active layers of the semiconductor structures, optimization of the device architecture and thus, the enhancement of the detection properties.

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From the X-ray diffraction analysis, the angular misorientation between discrete, homogeneous and perfect microblocks (~ 1 mm) varies from 5-10" to 20-30'. The estimated dislocation density within the small-angle boundaries varies from  $2 \times 10^6$  to  $8 \times 10^6$  cm<sup>2</sup>. The most perfect wafers with the lowest defect concentration (the estimated dislocation density ~  $2 \times 10^6$  cm<sup>2</sup>) were used for detector fabrication and further investigation.

# The Influence of Laser Surface Treatment **SRNL-STI-2020-00504** on Properties of CdTe X- and y-ray Detectors

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## X-RAY DIFFRACTOMETRY

The experimental investigations of CdTe wafers in different X-ray diffraction geometries (symmetrical 333, forbidden 222 reflections as well as asymmetrical one 331) using a Philips X'Pert PRO diffractometer were carried out. The simulation of reciprocal space maps (RSM) for (333) and (331) reflections have been performed using the model of a real crystal, which contains complexes of structural defects.

The influence of this system on the diffraction pattern is comparable to the set of edge dislocations with dislocation lines perpendicular to the surface plane and different directions of Burgers vector in this plane: a/2[10] and a/2[110]. The density of these dislocations was determined as 2.86  $\times$  10<sup>6</sup> cm<sup>-2</sup> and 2.38  $\times$  10<sup>6</sup> cm<sup>-2</sup>.



Reciprocal space maps of the most perfect and uniform sample,  $CuK_{\alpha 1}$ -radiation: a) (333) reflection, and b) (331) reflection



The least sample, entrance surface (111). X-ray scattering intensity distribution maps  $I_{h}(2\theta - \omega, \omega)$ (plotted in coordinates of reciprocal space  $I_h(q_x, q_y)$ , color online) at the reciprocal lattice node (333), Cu $K_{\alpha 1}$  -radiation: a) experimental RSM, b) calculated.





AFM-images of NiO film on CdTe single crystal substrates: a) before laser treatment; b) after laser treatment with an energy density of 2.4 J/cm<sup>2</sup>; c) after laser treatment with energy density of 3.6 J/cm<sup>2</sup>

Thus, using a laser treatment of Ni/CdTe and NiO/CdTe heterojunctions, both with respect to the substrate and the film, one can intentionally change their morphology and structure, and, accordingly, their electrophysical properties. This has decreased the dark reverse currents in Ni/CdTe and NiO/CdTe heterojunctions and improved the spectrometric characteristics of the detectors.

# **MORPHOLOGY AND STRUCTURE**

In order to modify and improve the structure and phase state of the Ni/CdTe and NiO/CdTe Schottky contacts, they were irradiated by an out-of-focus laser beam using a millisecond (1.5 ms) YAG-laser with 1.064 µm wavelength in the single pulse mode with an energy density of  $E = 2-4.5 \text{ J/cm}^2$ . The laser treatment modes were selected so that the threshold for melting or destruction of the material in the process of heating the surface and near-surface layers were not reached.

Due to the presence of a non-uniform temperature distribution in the area of laser beam and the gradient of thermoelastic stresses, structural and phase transformations in the Ni and NiO films under the action of the pulsed laser radiation take place.

The morphology and structure of the Ni and NiO films deposited on the surface of the CdTe:Cl crystals were studied by atomic force microscopy on NT-206 set. The AFM measurements were carried out in contact mode using CSC38/AL BS probe. The Ni metal film strongly absorbs the laser radiation by a system of free electrons. Therefore, the modification of the crystal is implemented in a relatively small surface layer of CdTe, which increases slightly with the power density of the laser beam.

> Due to the rapid heating in the Ni film, a significant increase in the size of the crystallites was observed from  $0.15 - 0.25 \,\mu m$  to 0.5-0.7 µm.

AFM images of Ni film on CdTe single crystal substrates: a) before laser treatment; b) after laser treatment with energy density of 3,6 J/cm<sup>2</sup>.

The NiO film is transparent to the laser wavelength at  $\lambda = 1.06 \ \mu m$ . Since the CdTe crystal is also transparent to  $\lambda = 1.06 \mu m$ , the laser irradiation energy absorption occurs predominantly on the inhomogeneities and defects in the crystal structure. However, the area of the effect of the laser on the CdTe crystal through the NiO film extends to a much greater depth than through the Ni film. It contributes to the redistribution and relaxation of defects and better phase homogeneity.

> A slight increase of crystallites size in NiO film from ~ 180 nm to ~ 230 nm is observed after laser treatment.





X-ray diffraction investigations of a set of CdTe wafers were carried out using a Philips X'Pert PRO diffractometer equipped with standard  $CuK_{\alpha 1}$  X-ray tube. The estimated dislocation density within the small-angle boundaries varies from  $2 \times 10^6$  to  $8 \times 10^6$  cm<sup>2</sup>.

## **DETECTOR CHARACTERISTICS**

### CONCLUSIONS

The surface morphology and structure of the Ni/CdTe and NiO/CdTe detectors were modified using a millisecond (1.5 ms) YAG-laser with 1.064 µm wavelength. The laser treatment of the heterojunctions, both with respect to the CdTe substrate and Ni and NiO film, can intentionally change the electrical properties and sensitivity of detectors.

Comparison of the I-V characteristics of the investigated Ni/CdTe and NiO/CdTe Schottky-diode heterostructures and well-known theoretical models have allowed us to explain the mechanisms of charge carrier transport and clarify the reasons limiting the use of the fabricated heterostructures as X- and  $\gamma$ -ray detectors.

The relatively low energy resolution of the detectors is attributed to the limitation of increasing the operating bias voltage because of an increase in the reverse dark current (leakage current). However, further improvement of the detecting properties can be achieved by modification of the conditions of contact deposition (optimization of the pre-treatments of *p*-CdTe crystals, change of the stoichiometric composition of Ni and NiO film, improvement of its structure, among other modifications).