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The structural disorder in $TlInS_2$ <Fe>

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Abstract

It is shown that the iron intercalation of layered crystals TlInS2 leads to the formation of nanolevels and nanoislands. Formed on the interlayer surface (001) $TlInS_2$ objects consist of nanoislands Fe, InS, $TlIn_9$, having a pyramidal shape and lead to structural disordering.

Keywords: *defects, structure, crystals, mass transfer, nano-objects, conductivity.*

1. Introduction

Compounds with diffuse phase transitions, which are often referred relaxors, are among the most intensively studied materials [1].

The interest in these compounds is determined by a combination of ferroelectric, piezoelectric properties and the ability to use these materials in a variety of devices of electronic equipment. In particular, optically transparent relaxors are an excellent medium for the accumulation of data, induced by light.

It is known that the properties of relaxors can be significantly changed with introduction of even small amounts of impurities which affect the charge state of the connections. In this case the shift of temperature maximum of dielectric constant can reach 50K or more. The temperature range in which the crystal lattice is observed instability of $TlInS_2$, very sensitive to the trivalent cation impurities having a different ionic radii and coordination numbers.

Currently $TlInS_2$ is one of the few semiconductor compounds in which there is a sequence of incommensurate and ferroelectric phase transitions (PT) [2-9]. The temperature dependence of the dielectric constant for crystals $TlInS_2$ doped with 0.1 at.% Cr, Mn, Yb, Sm, Bi, La. Constructed the dependence температуре phase transition of the ionic radius of the impurity atom.

It was found that Mn and Cr substitute In in the crystal lattice of $TlInS_2$, and Yb atoms, Sm, Bi, and La occupy octahedral voids in the tetrahedral complex of In_4S_{10}, creating internal pressure, which leads to a shift of phase transitions in high-temperature area.

The purpose of this work is to identify the different nanostructures on real surfaces (001) $TlInS_2$, intercalated Fe and cause structural disorder, creating local centers.

EXPERIMENTAL TECHNIQUE

Electron microscopic images were obtained on atomic force microscope (AFM) brand SOLVER NEXT. X-ray diffraction (XRD) studies of the surface were conducted on diffractometer company Philips Panalytical (HRD). Single crystals of $TlInS_2$, which are used for experiments were grown by the Bridgman method from the melt of non-stoichiometric composition and doped with iron.

In Figure. 1 and 2 represent the diffraction patterns of unalloyed $TlInS_2$ and intercalated by iron $TlInS_2$. In Figure. 3-4 are given the images of the surface (001) $TlInS_2$ <Fe> taken from AFM: the upper part of the image is directly AFM - the image of surface are given on the bottom of the distribution model were constructed on AUTOCAD program.

Particular interest to the nanoislands (NI), are small size (~ 500 nm), as clusters with a small number of bound states. Plates with surface orientation (001) cut from the samples. For studies chosen chipped along the base surface. Machining is not performed. Intercalation diffusion of atoms was carried out at 500K. The process of implementation (intercalation) along the wire layers at the temperature gradient T= 50 deg / sm.

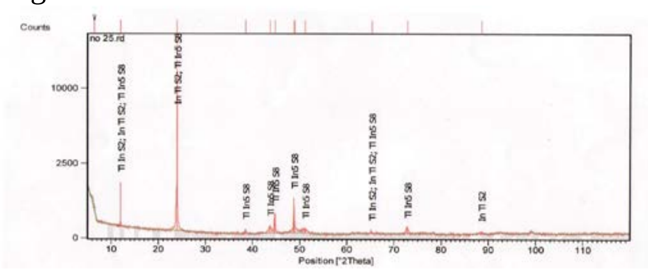

Fig.1. X-ray diffractogram single crystal of TlİnS$_2$. Along with reflexes TlİnS$_2$ at 2 $\theta=12^0$, 24^0 , $88,5^0$ and TlİnS$_8$ noticeable reflexes at 2 $\theta=12^0$, 235^0, 49^0, 65^0, $72,5^0$

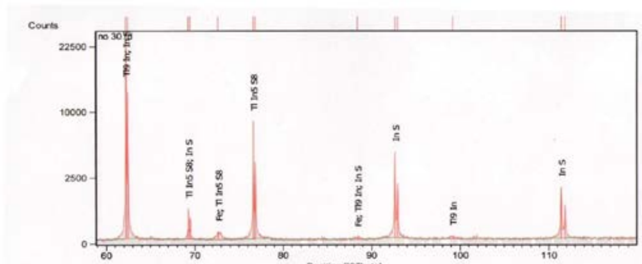

Fig.2 X-ray diffractogram of a single crystal intercalated with iron: formed from basic surface interlayer nanostructures following: of Fe at $2\theta=73^0$, $88,5^0$; İnS at 69^0, 88^0, 93^0, 112^0 Tlİn$_9$ 69^0, 88^0, 99^0.

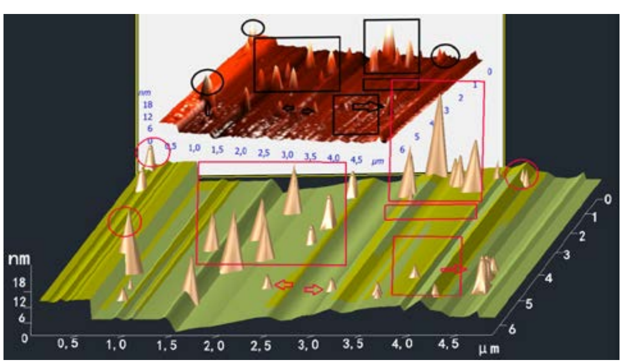

Fig.3 Upper part of the figure is the AFM image in 3D-scale cleaved surface TlInS$_2$ <Fe>; the lower part is the modeling of surface, which are clearly visible steps and NI (marked with ellipses), coagulated made of iron atoms (which are localized centers in highly defective TlInS2 <Fe-0,1% weight>).

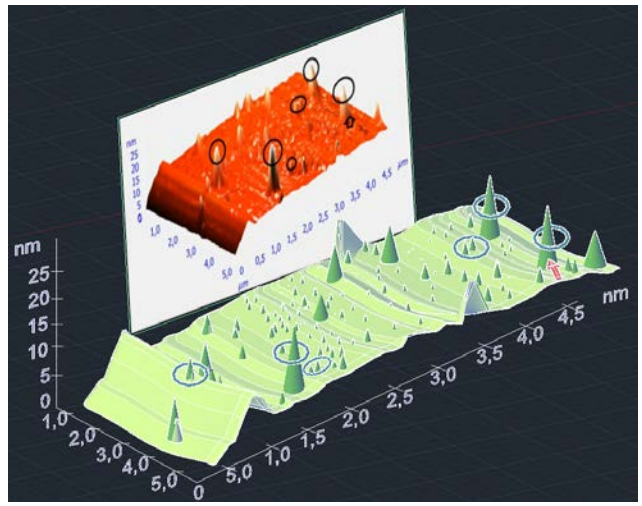

Figure 4. AFM images TlInS$_2$ <Fe-0,5% weight> aggregated by atoms Fe, İnS and Tlİn$_9$.

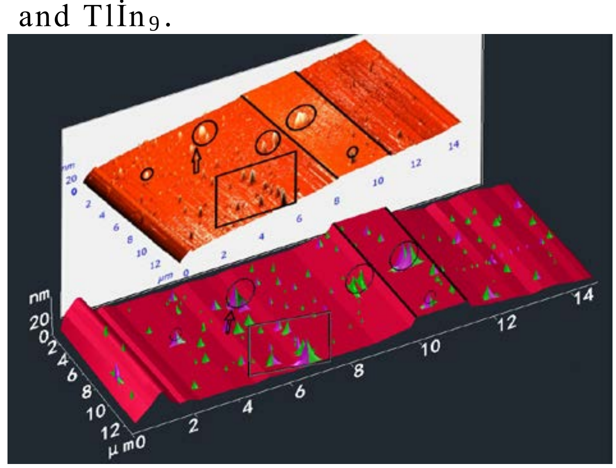

Figure 5. AFM images in 3D-scale TlInS$_2$ <Fe-0,5% weight> with NI and steps

DISCUSSION OF RESULTS

Consider the mass transfer in layered crystals type of TlInS$_2$, leading to the formation of nanoislands nanolevels and corrugated structures. Dislocation centers play a quantummechanical role in the localization and transfer of charge and heat in layered crystals. Studies have dangling bonds stages (fig.3-4) compounds of the surface showed their effect on the electronic structure. The formation of surface structures is required to mass transfer and plastic deformation, which has the character and regularities inherent in the organization of similar structures in other solid materials. The diffusion process is the main reason for the formation of periodic stage structures of nano objects Fe, InS and $TlIn_9$. In Figure. 3 squares marked congestion NI, NI marked individual by ellipses, arrows indicate the aggregated nanoislands. The surface consists of both atomically smooth areas and areas of coated micro steps with marked facet type nanoscale facets (Figure 3) located on the extended irregularities with a period (3-5), 10^2nm and 1-2 nm in height. At the bottom of Fig. 3-5 demonstrates the model AFM - micrographs of the surface of the interlayer with a regular system of terrace stages NI. The lines in Figure 5 marked sections highlight terrace as mesa structures. For all images bright regions correspond to protruding parts of the surface topography, dark colors corresponding recess. For all images bright regions correspond to protruding parts of the surface topography, dark colors corresponding recess. Dedicated nanoislands circles in Fig. 3-5 small clusters formed from the result of their coalescence around which will integrate arisen zones. Despite the low density of their distribution can be regarded as structural disorder centers, which charge localization occurs. The observed anomalies of the kinetic effects can be associated with these defects. The observed anomalies of the kinetic effects can be associated with these defects. Aggregate structure consisting of interlayer nanostructured elements can be connected to one another continuous chain of clusters that provide tunneling conductive channels, changing the properties of the crystal only along the axis "C". Thus, it is necessary to take into account the tunneling of electrons through an orderly closely spaced but also the interaction of the tunneling electrons with phonons.

Migration and the interaction of clusters with each other resulting in the formation of three-dimensional islands, wide terraces and corrugated structures.

Nanostructured self-organized processes occur in a restricted environment layer- chained crystal. The decisive here is the interlayer surface diffusion and incorporation of implanted atoms in favorable from an energy point of view the place. Since the spontaneous formation of ordered arrays but it turned energetically favorable, taking into account the effect of relaxation of residual stress surface, were obtained periodic structures (see. Fig. 3- 5) and NI. Study of the surface morphology and migration processes of atoms showed the formation stages with islands as result of the aggregation of the interlayer atoms and wide terraces. These defect structures fetus interaction point and volume defects.

CONCLUSION

It is shown that the intercalation of layered crystals $TlInS_2$ with iron leads in the formation of clusters in admixture $TlInS_2$ interlayer space. This allows us to consider the compound $TlInS_2$ like nanocomposite materials consisting of alternating layers of the original crystal and the introduced impurities. Formed on the interlayer surfaces $TlInS_2$ nano-objects are composed of Fe, InS, TlIn9 equilibrium with a pyramidal shape and characteristic of highly disordered systems. Discovered in the interlayer space NI and stages associated with the restructuring of the surface with an effective mass transfer between the base surfaces, through which the flow of heat. On the parameters of hopping conductivity inherent in these crystals will affect the density distribution detected nanostructures, which play the role of charge localization centers, and their composition on the energy level of these centers. Appropriate electrical effects in these crystals can be controlled via the metastable state at such centers.

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