STRUCTURAL FEATURES OF MANGANESE CONTAINING TOPOLOGICAL INSULATORS THE BASIS OF Bi_2Te_3

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Synthesis, crystal growth, X-ray examination of Mn-Bi-Te system compounds was carried out. It is shown that individual compounds with the general formulas $MnTe•nBi_2Te_3$ (where n = 1, 2, 3,...) crystallize in this system. The existence in this series of compounds of $MnBi_8Te_{13}$ (n = 4) and $MnBi_{10}Te_{16}$ (n = 5) is shown for the first time. In this work, the structural characteristics of the compounds of this homologous series are also given.

Keywords: Topological insulators, synthesis, crystal growth, X-ray diffraction
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Bi_2Te_3 has long been studied as one of excellent ambient-temperature thermoelectric materials. Recently, however, Bi_2Se_3 and Bi_2Te_3 have been of renewed interest because they are bulk topological insulators. Torological insulators (TIs) are insulators in bulk but show metallic conduction at the surface /1/. The conductive properties of the surface are a consequence of the strong spin-orbit interaction. The first experimentally discovered topological insulators were the $Bi_{1-x}Sb_x$ alloys. The same surface states were discovered in tellurides and selenides of bismuth and antimony: Bi_2Se3, Bi_2Te_3, Sb_2Te_3. In the seventies of the last century, the structures of Bi_2Te_3 crystals and many of its analogues were grown and solved. Authors showed that these crystals are layered and crystallize in the structural type of tetradymite. The contribution of the authors RM Imamov and SA Semiletov in the study of the crystal chemistry of these compounds was very large [2]. Almost forgotten these works after revealing their possession of the TI property again attracted the attention of scientists. So, Bi_2Te_3 is one of the most promising TIs. The blocks of this layered structure consist of quintuples of Te-Bi-Te-Bi-Te. Of particular interest have the influence of magnetic impurities and ferromagnetism on the topological surface states. The Bi_2Te_3 compound is a convenient matrix for the incorporation of magnetic impurities. It is shown that when the manganese is inserted up to nine percent, the structure of Bi_2Te_3 type is preserved /3/. We examined the interactions of Mn-Bi-Te elements with melting, at higher manganese contents. A further increase in concentration leads to the formation of structural blocks consisting of seven atomic layers. The first such compound consisting of seven-layer blocks (septuple) is $MnBi_2Te_4$. However, in the interval between Bi_2Te_3 and $MnBi_2Te_4$, several layered compounds with the general formula $MnTe • nBi_2Te_3$ (n = 1-5) are formed. It is not difficult to make sure that the number "n" corresponds to the number of quintuples located between septuples. Among these compounds, the $MnBi_2Te_4$ structure has already been refined. For the values n = 2 and 3, namely, for $MnBi_4Te_7$ and $MnBi_6Te_{10}$ their structural analogues are known.

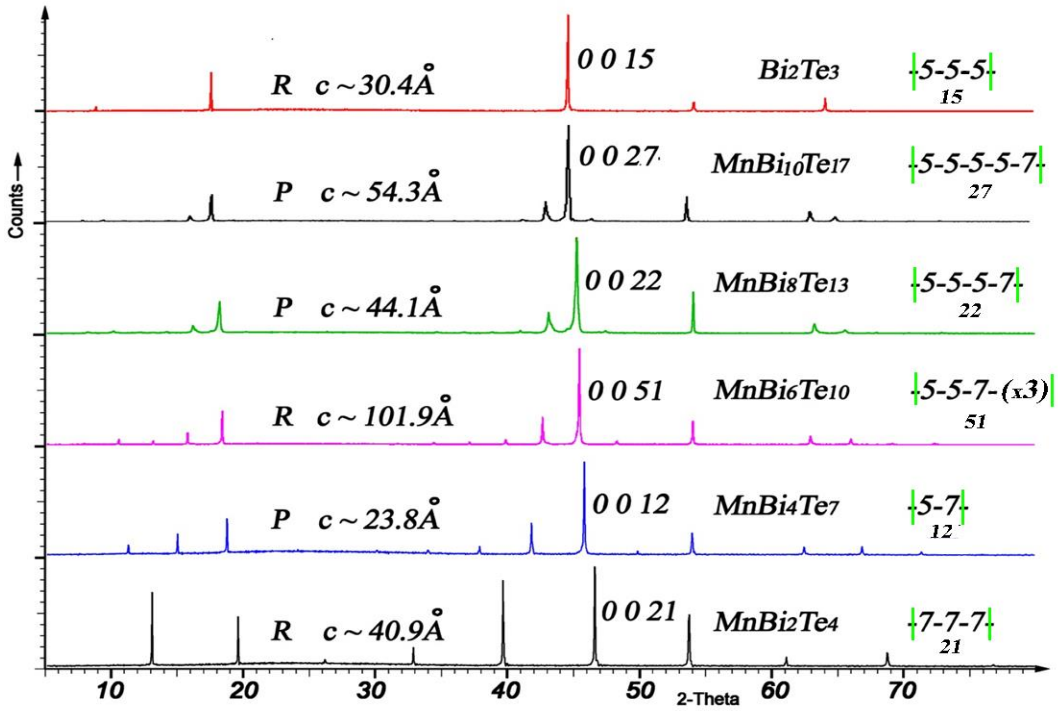

Fig.1. The diffraction patterns of $MnTe • nBi_2Te_3$ (n = 1-5) and Bi_2Te_3.

However, the formation of compounds with the compositions $MnBi_8Te_{13}$ (n = 4) and $MnBi_{10}Te_{16}$ (n = 5) for the first time we show. It should be noted that the growth of individual crystals of ternary phases of these compounds with dimensions of few millimeters for technologists is an impossible task. The main reason for this is the formation of a very stable MnTe phase at high temperatures. As a result of a long and painstaking work, we managed to isolate these phases in sizes of 1-3 mm. The fig 1 shows the diffraction patterns from cleaves of the selected crystals. In these pictures, reflexes like (00I) are visible, which allow us to determine the "c" parameters of these phases.

As can be seen from the fig 1, in all these compounds the strongest reflexes are in the 2-theta range of 44-47°. It is easy to verify that the values of the index ***l*** of these reflexes are equal to the number of atomic layers in one unit cell. Also, with a decrease in the relative amount of manganese in the composition, this peak shifts toward a decrease in the value of the 2-theta. It is clear that this is due to the difference in the ionic radii of the Mn and Bi atoms. As noted above, one cannot yet single-phase compounds of $MnBi_{2x}Te_{3x+1}$ formulations (x=1,2,...), but a mixture of several phases is always grown. Therefore, the determination of the exact positions of strong peaks in the range 2θ= 44-47° would unambiguously identify the phase composition of the sample.

X-ray diffraction analysis of the compounds $MnBi_2Te_4$ (n = 1) and $MnBi_4Te_7$ (n = 2) and $MnBi_6Te_{10}$ (n = 3) showed that in all these compounds the Te atoms are arranged in the cubic close packing type. Therefore, the value of the parameter c=44.1Å, shown in the fig 1 for $MnBi_8Te_{13}$ (n = 4), it is possible that it increases threefold. The fact is that the 22-layer structure cannot fit into a cubic package. Most likely, it will move into a 66-layer rhombohedral structure with the parameter c~132.3Å. However, additional studies are needed to confirm this.

The report will discuss the structural features of the above-mentioned crystals.

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[1] *Hai-Jun Zhang, Chao-Xing Liu, Xiao-Liang Qi, Xiao-Yu Deng, Xi Dai, Shou-Cheng Zhang, and Zhong Fang.* Electronic structures and surface states of the topological insulator $Bi_{1-x}Sb_x$. Phys. Rev. B 80, 085307, 2009

[2] *R. M. Imamov and S. A. Semiletov*, Kristallografiya, 15, No. 5, 972–978 (1970)

[3] *Y. S. Hor, et al*. Development of ferromagnetism in the doped topological insulator $Bi_{2-x}Mn_xTe_3$. Phys. Rev. B. 81, 195203 (2010)