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INVESTIGATIONS OF STACKING FAULTS AND POL1TYPE STRUCTURES IN MANGANESE DOPED ZnSe CRYSTALS OBTAINED FROM MELT PHASE

EDWARD MIcHALSKI, MIECZYSLAW DEMIANJUK, SLAWOMIR KAC.ZMAREK, JOZEF ZMIJA

Institute of Technical Physics
Military Academy of Technology
ul. Lazurowa, 00-908 Warszawa, Poland

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SUMMARY

THIS PAPER presents the results of X-ray investigations of stacking faults and politype structures in manganese doped ZnSe crystals obtained from the melt phase. The range of Mn concentration was established where the manner, in which the layers are set in the structure, varies. The single stacking faults at low dopant concentrations were investigated. The changes in layer settings under influence of Mn concentration were characterised by means of identification of politype structures 3C, 8H (44), 4H, 2H together with dependence of hexagonality of those structures on Mn concentration. The interpretation of results obtained is given based on the stacking faults energy SFE runs as a function of a structure hexagonality described in the previous work.

The exemplary distributions were obtained of politype structures along the ZnSe crystals heavily doped with manganese.

I. INTRODUCTION

THIS SHORT paper is, in its part dealing with politype structures, a continuation of the previous work, as well as of other works mentioned here. In its part dealing with the stacking faults this paper is a subsequent work, together with [1], on the subject of layer structures with low .concentration of stacking faults.

2. GENERAL CHARACTERISTICS OF CHANGES IN ZnSe CRYSTALS STRUCTURE UNDER THE INFLUENCE OF Mn IMPURITIES

The investigations were conducted in the manner identical as presented in the previous paper [2]. Fig. 1 shows composed rows of 10.1 X-ray diffraction photographs of crystals (rotated around the *c* axis) in the growing sequence of manganese concentration in samples tested. In the Mn concentration range below 6% by weight no changes in layer settings can be observed on X-ray diffraction photographs. In the 6—12% Mn range generally the hexagonal layers concentration increases with the increase in manganese contents. In the

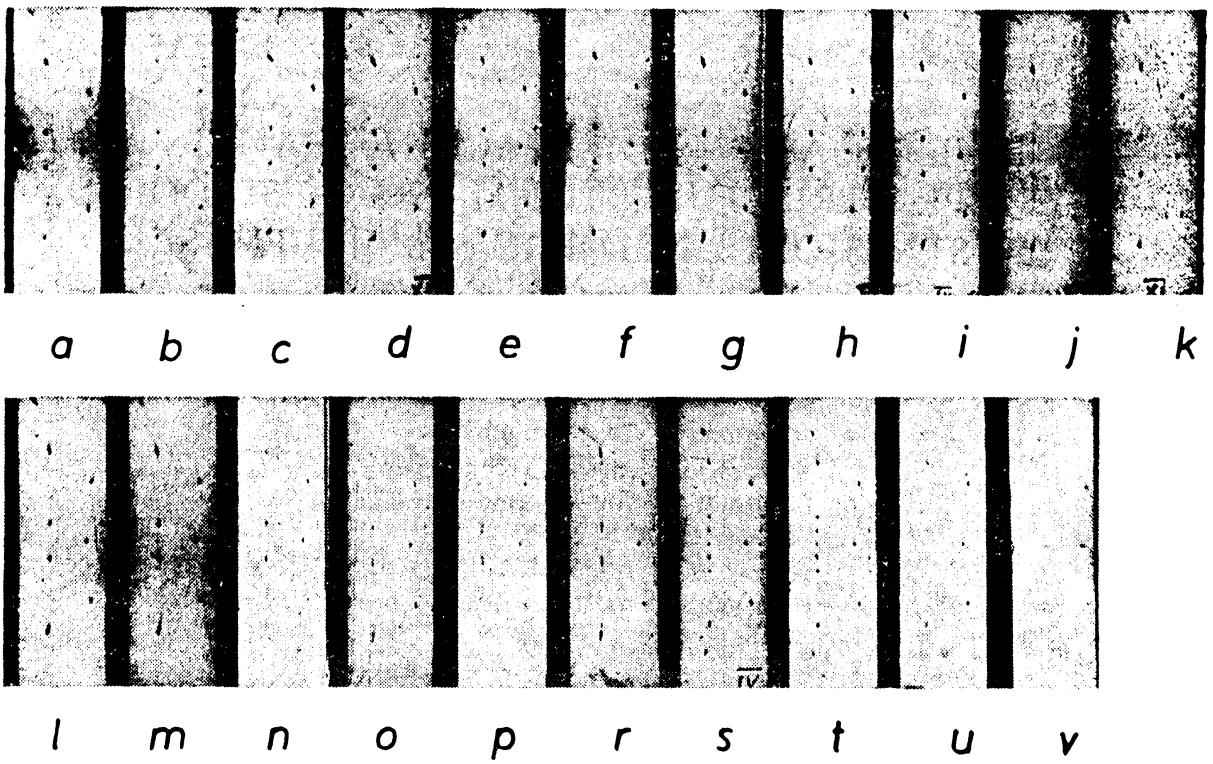

FIG. 1. Rows of 10.1 *X-ray* pictures of a rotated ZnSe crystal with the following Mn concentrations (in % by weight): a) 4.8 10^{-3}, b) 0.6, c) 3.7, d) 5.4-7.0, e) 5.7-6.7, 0 5.6-7.8, g) 6.3-7.2, h) 6.3-7.3, i) 6.3-7.3, j) 6.3-7.3. k) 5.9-7.5, 1) 6.6-7.6, m) 6.8-9.6, n) 7.7-10.1, o) 7.7-10.1, p) 7.7-10.1, r) 7.7-10.1, s) 9.1-10.1, t) 9.9-10.9, u) 10.3-11.3, v) 11.5-12.5.

order of increasing Mn contents the following structures appear sequentially: 3C, 3C+DS, 8H+DS, 4H+DS, 2H. Above 12% of Mn only the 2H structure is observed and the increase in Mn contents does not influence stacking of layers in the structure.

3. STACKING FAULTS IN CRYSTALS AT LOW IMPURITY CONCENTRATIONS

The investigations of stacking faults were conducted by means of Laue method using the microlamp. The light beam illuminated the area of about 5 mm. The distance between crystal and film was 4 cm. The photographs were taken from the surface obtained by splitting the ((110)) type surface. Fig. 2a shows the Laue pattern with the reflexions indexed. Fig. 2b shows the blow-out of a reflexion with two systems of lines (caused by stacking faults) visible, that form an angle of 54°44' in the photograph plane. In order to interpret such pictures the directions of particular lines should be considered together with the distribution of reflexions without those lines. The line direction usually agrees with the direction of stacking faults plane trace. On the other hand those lines do not appear on the reflexions distributed along the stacking faults plane trace and symmetrically on its sides. This results from the reflexions being common for both sequences of layer settings, the proper one and the one changed by the stacking fault. This feature may be used for determining the location of stacking faults plane. In this manner it was found out, in case of faults responsible for longer lines (that spread along the whole spectrum), that

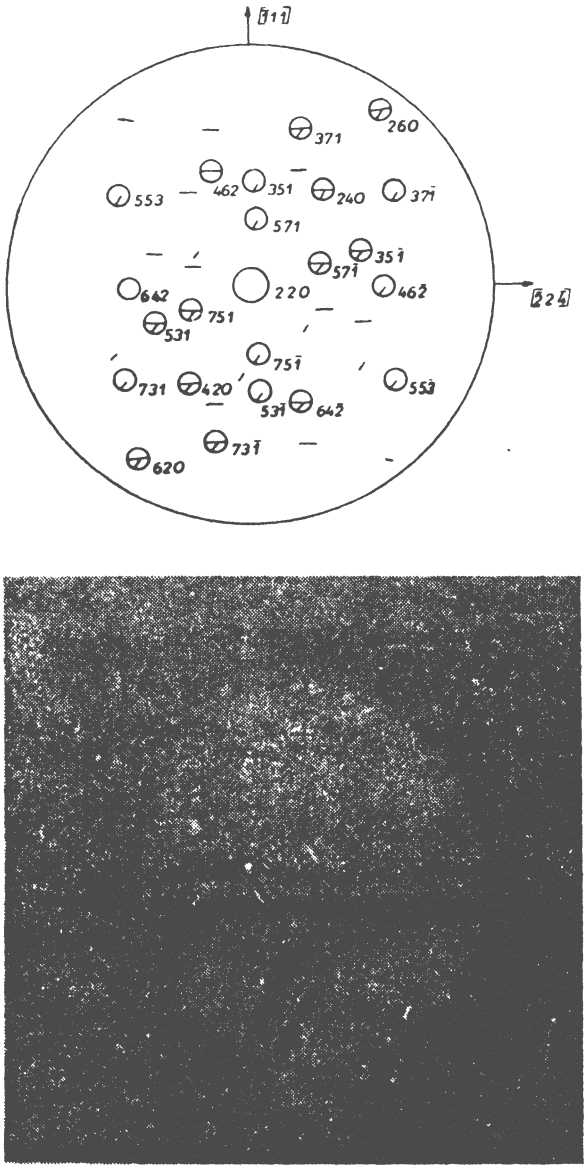

FIG. 2. a) The Laue pattern photograph, b) 620 reflection, magnified 6 times.

the plane trace of those faults is defined by the 462 and 642 reflexions. According to the stereographic projection (Fig. 3) this is the (1̲11) plane. Those stacking fault lines are not observed on the 351, 53̲1, 571, 75̲1 reflexions due to symmetrical distribution of reflexions from the planes of the same type relative to the (1̲l1) plane. Similarly those lines are not observed on the 553, 55̲3, 731 and 37̲1 reflexions due to almost symmetrical distribution of wide reflexion pairs from various planes: 553-731 and 37̲1-553 relative to the (1̲11) plane.

Shorter lines on the Laue pattern fall along the [[110]] type direction. The reflexions 642 and 462, that do not exhibit those lines, are not distributed along plane trace of those stacking faults. No mutually complementing reflexion parts appear symmetrically on both sides of plane trace defined by 642 and 462 reflections. The plane trace of those stacking faults defines the direction of shorter lines together with the condition that for the 642 and 462 reflexions exist other reflexions from the ((642)) type planes symmetrical relative to this plane. This condition is fulfilled by the (111) plane, which is marked on

the stereographic projection (Fig. 3) with the continuous line. The poles of ((462)) type planes situated symmetrically relative to the (111) plane are connected with dotted lines on Fig. 3.

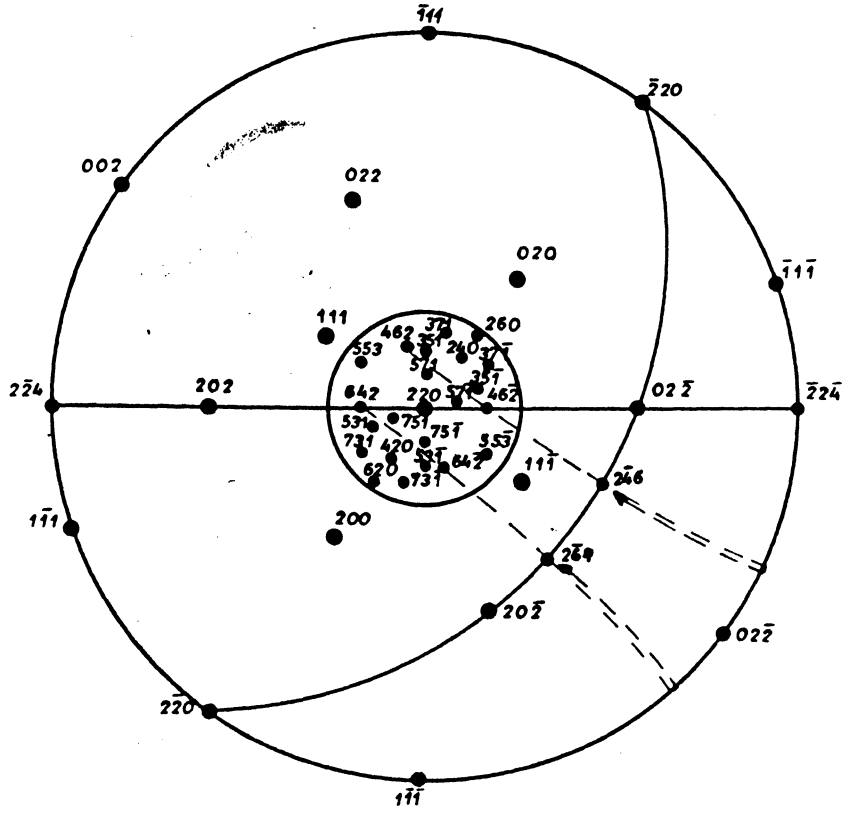

FIG. 3. Stereographic projection of the regular face-centered system with marked stacking faults in (he crystals tested.

For a better spatial presentation of stacking faults existing in the crystal tested Fig. 4 shows the perspective picture of an elementary cell with stacking faults planes marked, together with the projection of such a cell on the (110) plane.

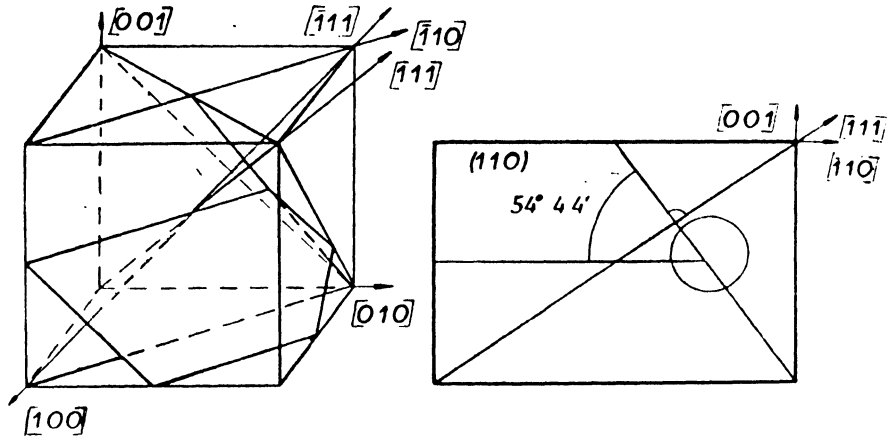

FIG. 4. Spatial picture of elementary cell of crystal tested with marked stacking faults planes and the picture of their traces on the (110) plane. The *X*-ray beam was covering the circled area.

Since in pure ZnSe crystals obtained with the same method no existence of stacking faults was found, the impurities may be considered the reason for their appearance. Moreover, the structure of defects shows that in the initial period of stacking faults growth in the crystal none of the [[111]] type directions is distinguished as the direction of the future *c* axis of polytype structures. This may give ground to reasoning that the polytypism phenomenon is not decided upon by temperature gradients, stresses or any other vector type physical quantity.

4. IDENTIFICATION OF THE 8H POLITYPE ELEMENTARY CELL

The 8H politype structure is rarely found in crystals of other $A^{II}B^{VI}$ compounds or in crystals with other type of doping. For example in the very comprehensive investigations by KOZIELSKI [3] no single case was found. Moreover, no reports in literature exist about the correlation between occurrence of 8H structures and the impurity contents or heating temperature for any other crystals. Fig. 5 shows *X*-ray diffraction photographs of crystals rotated around the *c* axis with 10.1 order reflexions indexed. This is the *X*-ray diffraction photograph of the 8H politype since it shows the hexagonal lattice and periodicity of 8.

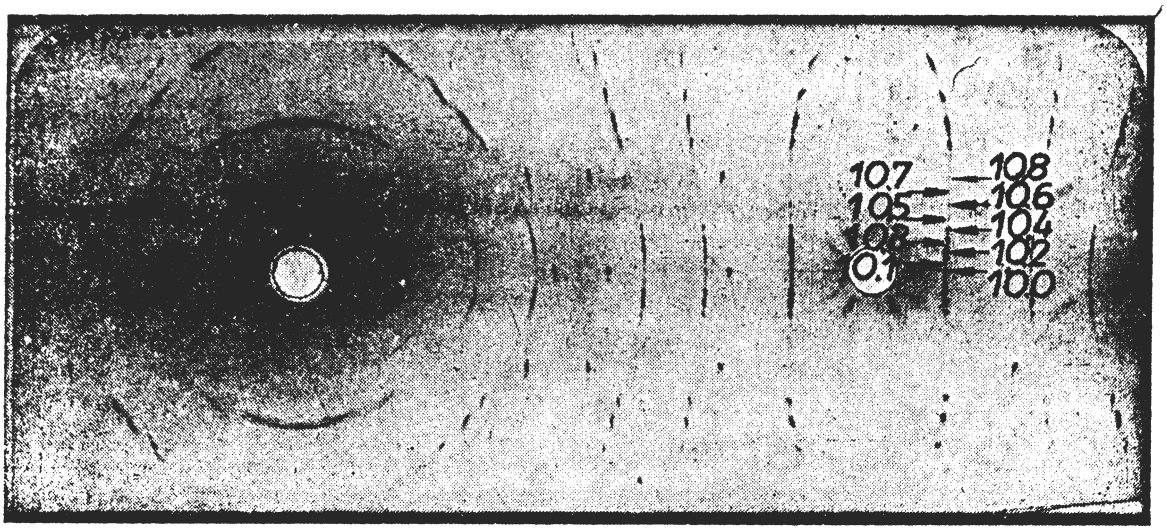

FIG. 5. *X*-ray diffraction photograph of the 8H politype tested.

TABLE 1
Theoretical intrinsings of reflexion for various politype 8H and results of measurements

hkl	10.0	10.1	10.2	10.3	10.4	10.5	10.6	10.7	10.8
(44)	143	67	885	1000	194	44	39	12	50
(3311)	189	821	389	1000	598	44	17	146	66
(71), (17)	717	544	670	1000	323	527	228	228	251
3212, 2123	246	915	965	817	1000	34	46	146	86
politype tested	150	70	900	1000	200	50	50	10	60

The manner in which the layers set in the elementary cell of politype was determined by comparing the relative intensities of 10.1 order reflexions observed with those calculated from all possible layer settings in the eight-layered hexagonal elementary cell. Those results are collected in Table 1. Based on those results it is easy to conclude that the observed structure is of 8H type (44).

5. EXPERIMENTAL RUN AND INTERPRETATION OF α DEPENDENCE ON c BASED ON THE GENERALIZED PLOT OF SFE = $f(\alpha)$

The analysis of not completely arranged structures was made using the model analysis method. The dependence of hexagonality α on dopant concentration obtained is shown on Fig. 6. When comparing this plot with those obtained for ZnS crystals one may notice

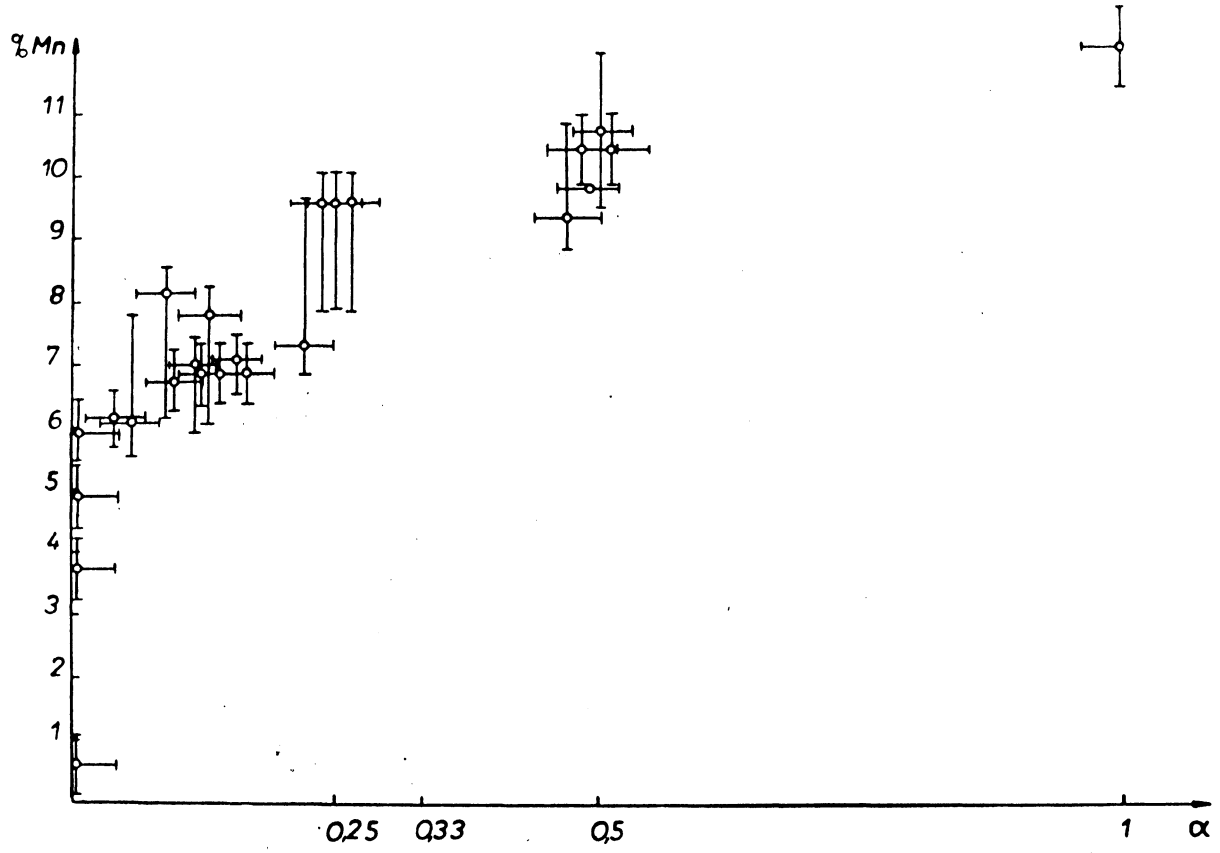

FIG. 6. Experimental dependence of hexagonality on the Mn concentration in ZnSe.

the same character of plots. The basic difference between the plots consists in the shift of the ZnSe plot along the dopant concentration axis by 6%. When interpreting the results based on the SFE = $f(\alpha)$ function one must consider the SFE range corresponding to the Mn contents of 0 to 6% as energy necessary for driving the ZnSe crystal to the state where its structure depends on the increase of impurity contents. In this respect the ZnSe crystals case may be considered more general than the ZnS crystals case.

6. THE DISTRIBUTION OF POLITYPE STRUCTURES ALONG THE ZnSe CRYSTALS HEAVILY DOPED WITH Mn

It was found that along such crystals the impurity concentration may change in the range sufficient for development of significant structural differences. Fig. 7 illustrates such exemplary distribution of polytype structures (4H, 3C+DS, 8H+DS, 3C+DS) along the ZnSe crystal.

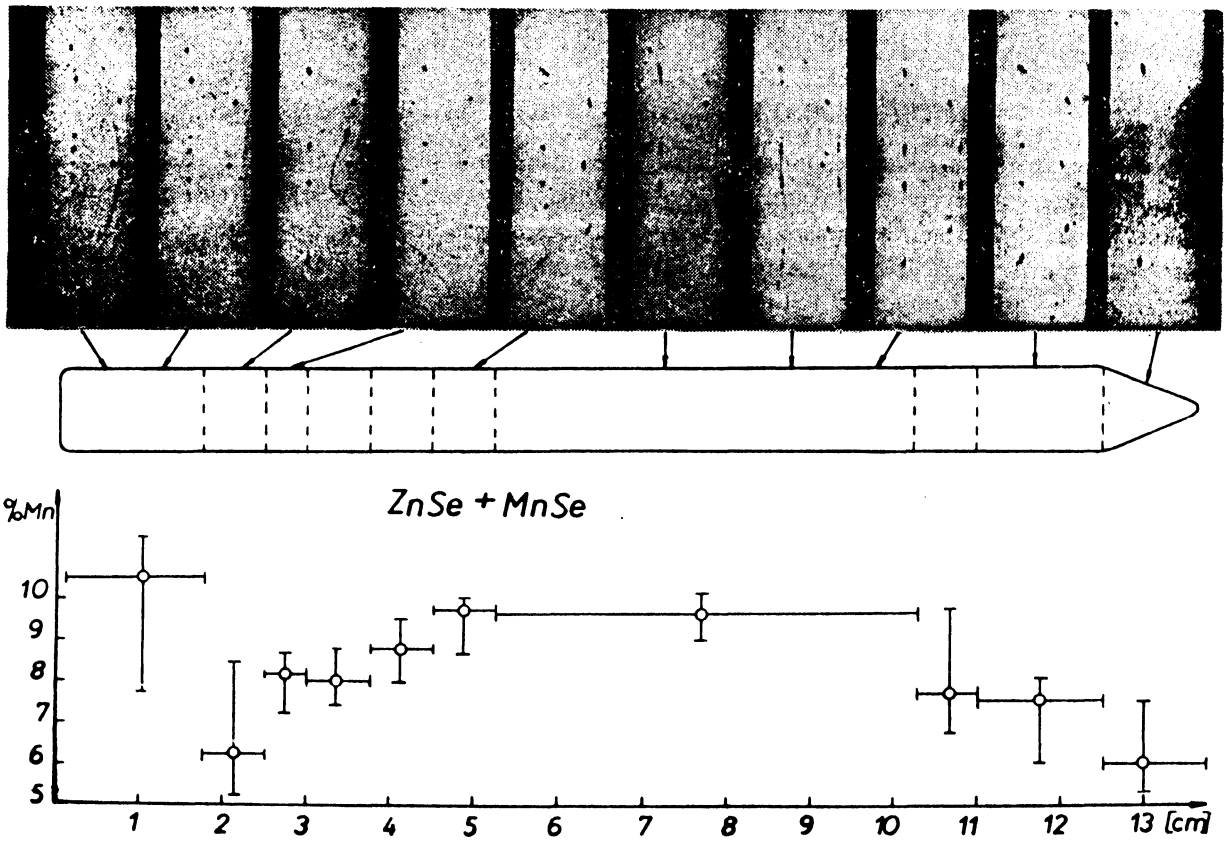

FIG. 7. Structures distribution along the ZnSe + MnSe crystal.

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STRESZCZENIE

BADANIA BŁĘDÓW UŁOŻENIA I STRUKTUR POLITYPOWYCH W DOMIESZKOWANYCH MANGANEM KRYSZTALACH ZnSe OTRZYMYWANYCH Z FAZY STOPIONEJ

W pracy przedstawiono wyniki rentgenograficznych badań błęd6w ułożenia i struktur politypowych w domieszkowanych manganem kryształach ZnSe otrzymywanych z fazy stopionej. Stwierdzono w jakim zakresie koncentracji Mn zmienia się spos6b ułożenia warstw w strukturze. Zbadano pojedyncze błędy ułożenia przy małych koncentracjach domieszki. Scharakteryzowano zmiany w ułożeniu warstw pod

wpływem domieszek Mn poprzez identyfikację struktur politypowych **3C,** 8H (44), 4H, 2H oraz zależność heksagonalności tych struktur od koncentracji Mn. Podano interpretację otrzymanych wyników opierając się na metodzie analizy przebiegu energii błędów ułożenia struktur (SFE — stacking faults energy) w funkcji heksagonalności, omówioną w poprzedniej pracy. Zbadano przykładowe rozkłady struktur politypowych wzdłuż kryształów ZnSe silnie domieszkowanych manganem.

РЕЗЮМЕ

ИССЛЕДОВАНИЕ ОШИБОК УПАКОВКИ И ПОЛИТИПОВЫХ СТРУКТУР В ЛЕГИРОВАННЫХ МАРГАНЦЕМ КРИСТАЛЛАХ ZnSe, ПОДУЧИВАЕМЫХ ИЗ СПЛАВЛЕННОЙ ФАЗЫ

В работе представлены результаты рентгенографических исследований ошибок упаковки и политиповых структур в легированных марганцем кристаллах ZnSe подучиваемых из сплавленной фазы. Обсужден диапазон концентрации марганца, в котором изменяется способ упаковки слоев в структуре. Исследовано одиночные ошибки упаковки при небольшой концентрации примеси. Определены изменения в упаковке слоев под влиянием примесей Мп через идентификацию политиповых структур 3С, 8Н (44), 4Н, 2Н, а также зависимость гексагональности этих структур от концентрации Мп. Представлено интерпретацию полученных результатов, опираясь на анализе энергии ошибок упаковки структур (SFE — stacking faults energy) в функции гексагональности обсужденной в предыдущей работе. Расследованы примерные распределения политиповых структур вдоль кристаллов ZnSe сильно легированных марганцем.