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INTRINSIC STACKING FAULT IN SINGLE CRYSTALS OF In_XMoSe_2 $(0 \le X \le 1)$

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The crystals of In_xMoSe_2 $(0 \le x \le 1)$ have been grown by a direct vapour transport technique. The structural characterizations of these crystals are made by XRD method. The particle size for a number of reflections has been calculated using the Scherrer's formula. There are considerable variations are shown in deformation (α) and growth (β) fault probabilities in In_xMoSe_2 $(0 \le x \le 1)$ single crystal due to off-stoichiometry, which possesses the stacking fault in the single crystal. The opposite sign of both probabilities are indicated that, the created stacking fault is of intrinsic type.

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1. Introduction

The perfect crystals are not available in nature or fabricated in laboratory, it is an ideal concept. There are several types of defects are present in crystal e.g. point defects, stacking fault etc. The study of stacking fault is made either by electron microscope or by X-Ray diffraction method [1, 2]. During recent years, transition metal dichalcogenides (TMDC) of group IV-b,V-b and VI-b have received considerable attention because of their uses particularly as electrodes in photoelectrochamical (PEC) solar ce1l for conversion of solar energy into electrical energy as well as photonic devices in various electronic applications [1-6]. The compounds crystallize in quasi-two-dimensional layer structure consisting of chalcogenes, which are held together by relatively weak Van der Waal's forces. Because of these weak Van der Waal's forces between the layers, facilitates to intercalate foreign atoms, ions or neutral molecules to form new compounds [1-6]. Intercalated compounds of disulphide and diselenide of molybdenum and tungsten have been extensively studied by various researchers. These crystals become superconducting when intercalated with alkali and alkaline earth metals [1-6]. The study of stacking fault is very important one, because it plays an important role in the description of defects. The conversion behaviour of a solar cell is closely related to the perfection of the electrode material and since stacking fault play a fundamental role in the description of defects structure, therefore their study is of both practical and theoretical interest [2]. The enhanced conduction of the stacking fault along the c-axis is difficult to understand because of the extreme two-dimensional characters of the layered compounds of $MoSe_2$ and its intercalated compounds of i.e. In_xMoSe_2 $(0 \le x \le 1)$. The only way to understand this conduction is by supposing the presence of stacking faults in these crystals. It is clear from the literature survey that, the research work on intercalated compounds of

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$MoSe_2$ is almost negligible. Hence, it was decided to work on In_xMoSe_2 $(0 \le x \le 1)$ single crystals [1-6].

2. Experimental details

For the X-Ray diffraction work, several small crystals from each group were finely ground with the help of an agate mortar and filtered through 106 micron sieve to obtain grains of nearly equal size. X-Ray powder patterns were recorded on Philips generator using Cukα radiation. The X-ray diffractograms of $InxMoSe_2$ $(0 \le x \le 1)$ single crystals are narrated in our earlier paper [1]. The input parameters, which are taken from the X-Ray diffractograms of each crystal, are tabulated in Table 1, which are used in present calculation.

Table 1. Input parameters, which are used in present calculation.

hkl values	$In_{0.25}MoSe_2$			$In_{0.50}MoSe_2$			$In_{0.75}MoSe_2$			$InMoSe_2$		
	d - values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle ^{0} (2θ)	*d* - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle ^{0} (2θ)	*d* - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle ^{0} (2θ)	*d* - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle ^{0} (2θ)
102	2.6158	0.080	34.255	2.6111	0.140	34.315	2.6082	0.080	34.395	2.6097	0.240	34.335
103	2.3774	0.060	37.810	2.3756	0.080	37.840	2.3756	0.120	37.840	2.3774	0.080	37.810
105	1.9152	0.100	47.430	1.9112	0.080	47.535	1.9147	0.080	47.445	1.9171	0.080	47.380

The formulae of deformation and growth probabilities, which are given by Warren [7] as follows

$$B_{2\theta} = \frac{360 \tan\theta}{\pi^2} l \left(\frac{d}{c}\right)^2 (3\alpha + 3\beta),$$

for l even (1)

and

$$B_{2\theta} = \frac{360 \tan\theta}{\pi^2} l \left(\frac{d}{c}\right)^2 (3\alpha + \beta),$$

for l odd (2)

where $B_{2\theta}$ denotes the full width at half the maximum intensity, d is the hkl spacing, c is equal to $2d_{002}$, α and β are the deformation fault probability and the growth probability. The presently calculated values of α and β are shown in Table 2. All the calculations are performed for (102), (103) and (105) reflections.

Table 2. Presently calculated values of stacking fault probabilities.

Stacking fault probability	$In_{0.25}MoSe_2$	$In_{0.50}MoSe_2$	$In_{0.75}MoSe_2$	$InMoSe_2$
α	0.0025037	0.0026711	0.0023574	0.0033694
β	-0.0024799	-0.0026637	-0.0023324	-0.0033157

3. Results and discussion

From the study of Table 2, it is seen that there is a significant variation shown in the deformation fault probability (α) and growth probability (β) due to off-stoichiometry i.e. composition of Indium in the MoSe2 single crystal. The variation of stacking fault i.e. both probabilities is due to the creation of the defects in the crystal. The values of α and β are nearly of the same order. But opposite sign of both probabilities are indicated that, the created stacking fault is an intrinsic type because, existence of such stacking fault leads to a localization of electron states and will provide possibility of conduction with increasing amount of indium can once again be explained in terms of the increase in the charge carriers i.e. electrons, which is the resultant of the enhanced amount of indium in $InxMoSe_2$ $(0 \le x \le 1)$. Any proof of such types of calculation is not available in the literature so that it is difficult to compare our results with them and write any strong remarks. The calculation of the stacking fault may be considered as one of the guidelines for further detailed study of defects and various properties of crystals.

It was shown by Cockyne et al. [8] that significant improvement in resolution of the structure of lattice defects could be obtained from dark field electron micrographs taken in weakly diffracted beams. Ray and Cockyne [9], using the weak beam technique, directly observed splitting of dislocations into partials of Si. Since then several investigators [10-14] and most recently Mao and Knowles [15] have observed dissociation of lattice dislocations into partials. The presence of stacking faults has been recently shown in WS_2 single crystals by Agarwal et al. [16]. All these investigators have used the spacing between partials to estimate the stacking fault energy. Gross and Teichler [17] formulated a real space method, Kenway [18] atomic lattice stimulation and Xiliang et al. [19] a method based on improved embedded-atom method for theoretical estimation of stacking fault energies in different materials. All these estimations when compared with SFE measurements made using weak beam techniques show a favourable agreement.

The low values of stacking fault probabilities allows for easy gliding on the basal plane of $InxMoSe_2$ $(0 \le x \le 1)$ layers thus leading to easy creation of stacking faults and its excellent properties as solid lubricating agent [16].

4. Conclusion

X-ray diffractogrms have clearly mentioned that the difference in InxMoSe2 $(0 \le x \le 1)$ single crystals due to off-stoichiometry. The analysis of deformation fault probability (α) and growth probability (β) of $InxMoSe_2$ $(0 \le x \le 1)$ single crystals has shown that indium intercalation affects the stacking fault in the single crystals. Also the opposite signs of both probabilities are indicated that, the created stacking fault is of intrinsic type in nature.

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