



STACKING FAULTS IN THE SINGLE CRYSTALS

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Abstract

The single crystals of In_xMoSe_2 ($0 \leq x \leq 1$) and Re-doped MoSe_2 viz. $\text{MoRe}_{0.005}\text{Se}_{1.995}$, $\text{MoRe}_{0.001}\text{Se}_{1.999}$ and $\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$ have been grown by a direct vapour transport technique (DVT) in the laboratory. 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 ($0 \leq x \leq 1$) and Re-doped MoSe_2 single crystals due to off-stoichiometry, which possesses the stacking fault in the single crystal.

Key words: In_xMoSe_2 , single crystals, XRD, particle size, deformation probability, growth probability, stacking fault.

I. 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. 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 photoelectrochemical (PEC) solar cell for conversion of solar energy into electrical energy as well as photonic devices in various electronic applications. 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, facilitate to intercalate foreign atoms, ions or neutral molecules to form new compounds. 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 [1-19]. 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. 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 In_xMoSe_2 ($0 \leq x \leq 1$) and Re-doped MoSe_2 compounds viz. $\text{MoRe}_{0.005}\text{Se}_{1.995}$, $\text{MoRe}_{0.001}\text{Se}_{1.999}$ and $\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$. The only way to understand this conduction is by supposing the presence of stacking faults in these crystals. Recently, we have reported some properties of such materials [1-15]. Very recently Sumesh *et al.* [16, 17] have been reported specific contact resistance at In-n MoSe_2 interfaces and current-voltage-temperature characteristics experimentally. The stacking fault energy of

various compounds has been studied by various researchers [18-31]. It is clear from the literature survey that, the research work on the stacking fault of the compounds of MoSe_2 is almost negligible. Hence, it was decided to work on In_xMoSe_2 ($0 \leq x \leq 1$) and Re-doped MoSe_2 viz. $\text{MoRe}_{0.005}\text{Se}_{1.995}$, $\text{MoRe}_{0.001}\text{Se}_{1.999}$ and $\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$ single crystals.

II. 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 $\text{CuK}\alpha$ radiation. The X-ray diffractograms of In_xMoSe_2 ($0 \leq x \leq 1$) and Re-doped MoSe_2 viz. $\text{MoRe}_{0.005}\text{Se}_{1.995}$, $\text{MoRe}_{0.001}\text{Se}_{1.999}$ and $\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$ single crystals are narrated in our earlier paper [1-15]. The input parameters, which are taken from the X-Ray diffractograms of each crystal, are tabulated in Tables 1-3, used in present calculation.

Table 1: Input parameters of In_xMoSe_2 ($0 \leq x \leq 1$) single crystals.

<i>hkl</i> values	$\text{In}_{0.25}\text{MoSe}_2$			$\text{In}_{0.50}\text{MoSe}_2$		
	<i>d</i> - values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle (2θ) ($^\circ$)	<i>d</i> - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle (2θ) ($^\circ$)
102	2.6158	0.080	34.255	2.6111	0.140	34.315
103	2.3774	0.060	37.810	2.3756	0.080	37.840
105	1.9152	0.100	47.430	1.9112	0.080	47.535

Table 2: Input parameters of In_xMoSe_2 ($0 \leq x \leq 1$) single crystals.

<i>hkl</i> values	$\text{In}_{0.75}\text{MoSe}_2$			InMoSe_2		
	<i>d</i> - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle (2θ) ($^\circ$)	<i>d</i> - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle (2θ) ($^\circ$)
102	2.6082	0.080	34.395	2.6097	0.240	34.335
103	2.3756	0.120	37.840	2.3774	0.080	37.810
105	1.9147	0.080	47.445	1.9171	0.080	47.380

Table 3: Input parameters of Re-doped single crystals.

<i>hkl</i> values	$\text{MoRe}_{0.005}\text{Se}_{1.995}$			$\text{MoRe}_{0.001}\text{Se}_{1.999}$			$\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$		
	<i>d</i> - values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle (2θ) ($^\circ$)	<i>d</i> - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle (2θ) ($^\circ$)	<i>d</i> - Values (Å)	Peak Intensity counts ($\beta_{2\theta}$) (s^{-1})	Angle (2θ) ($^\circ$)
102	2.6158	0.080	34.255	2.6111	0.140	34.315	2.6082	0.080	34.395
103	2.3774	0.060	37.810	2.3756	0.080	37.840	2.3756	0.120	37.840
105	1.9152	0.100	47.430	1.9112	0.080	47.535	1.9147	0.080	47.445

The formulae of deformation and growth probabilities, which are given by Warren [18] as follows:

$$B_{2\theta} = \frac{360 \tan \theta}{\pi^2} l \left(\frac{d}{c} \right)^2 (3\alpha + 3\beta), \quad \text{for } l \text{ even} \quad (1)$$

and

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

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 Tables 4 and 5. Most of all calculations are performed for (102), (103) and (105) reflections.

III. RESULTS AND DISCUSSION

From the study of Tables 4 and 5, 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 MoSe_2 and Re-doped MoSe_2 viz. $\text{MoRe}_{0.005}\text{Se}_{1.995}$, $\text{MoRe}_{0.001}\text{Se}_{1.999}$ and $\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$ single crystals. 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 found nearly of the same order. Any theoretical or experimental 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.

Table 4: Stacking fault probabilities of In_xMoSe_2 ($0 \leq x \leq 1$) single crystals.

Stacking fault probability	$\text{In}_{0.25}\text{MoSe}_2$	$\text{In}_{0.50}\text{MoSe}_2$	$\text{In}_{0.75}\text{MoSe}_2$	InMoSe_2
α	0.0025037	0.0026711	0.0023574	0.0033694
β	0.0025299	0.0027837	0.0022524	0.0032857

Table 5: Stacking fault probabilities of Re-doped MoSe_2 single crystals.

Stacking fault probability	$\text{MoRe}_{0.005}\text{Se}_{1.995}$	$\text{MoRe}_{0.001}\text{Se}_{1.999}$	$\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$
α	0.0025037	0.0026711	0.0023574
β	0.0024799	0.0026637	0.0023324

It was shown by Cockyne *et al.* [19] 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 [20] have used weak beam technique, directly observed splitting of dislocations into partials of Si. Since then several investigators [21-25] and most recently Mao and Knowles [26] have observed dissociation of lattice dislocations into partials. The presence of stacking faults has been studied by Agarwal *et al.* [27, 28] in WS_2 , $\text{WS}_{1.8}$ and WSe_2 single crystals. All these investigators have used the spacing between partials to estimate the stacking fault energy. Gross and Teichler [29] formulated a real space method, Kenway [30] atomic lattice stimulation and Xiliang *et al.* [31] 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 In_xMoSe_2 ($0 \leq x \leq 1$) and Re-doped MoSe_2 viz. $\text{MoRe}_{0.005}\text{Se}_{1.995}$, $\text{MoRe}_{0.001}\text{Se}_{1.999}$ and $\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$ layers thus leading to easy creation of stacking faults and its excellent properties as solid lubricating agent.

IV. CONCLUSION

X-ray diffractograms have clearly mentioned that the difference in In_xMoSe_2 ($0 \leq x \leq 1$) and Re-doped MoSe_2 viz. $\text{MoRe}_{0.005}\text{Se}_{1.995}$, $\text{MoRe}_{0.001}\text{Se}_{1.999}$ and $\text{Mo}_{0.995}\text{Re}_{0.005}\text{Se}_2$ single crystals due to off-stoichiometry. The analysis of deformation fault probability (α) and growth probability (β) of all the single crystals has shown that indium intercalation and Re-doping affects the stacking fault probabilities. The experimental proof is not available in the literature but, the present investigation provides an important set of data for most of the single crystals which can be very useful for further comparison either with theory or experiment. Such study on the stacking fault of other single crystals is in progress.

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