

Effect of Concentration of the Electrolyte on the performance of Photoelectro Chemical (PEC) Solar Cell using $\text{MoTe}_{1.5}\text{Se}_{0.5}$ Single Crystal

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Abstract: The single crystal of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ grown by chemical vapour (CVT) transport technique is used for the fabrication of Photoelectro chemical (PEC) solar cells. The effect of the concentration of the electrolyte on the conversion efficiency of the fabricated PEC solar cell is studied.

Keywords: Single crystal of $\text{MoTe}_{1.5}\text{Se}_{0.5}$, Photoelectrochemical solar Cell, Effect of concentration of the Electrolyte, conversion efficiency

1. Introduction

The transition metal dichalcogenides (TMDCs) materials have considerable importance because of their usefulness as lubricating materials, switching devices, electrodes for photoelectrochemical solar cells, etc. The chemical vapour transport (CVT) techniques using halogen (Br or I) as the transporting agent has been found to be a suitable technique by several researchers [1-7] for growing the single crystals of layered compounds. It appears from the literature that there has been no previous attempt to grow the single crystals of $\text{MoSe}_x\text{Te}_{2-x}$ ($0 \leq x \leq 2$). Kline et al[8] reported that the transition metal dichalcogenides (TMDCs) form a wide range of solid solutions[9,10] with either mixed metal or chalcogenide composition or both and the properties, like crystal structure, band gap, band positions and stability to corrosion, which are of prime interest to photoelectrochemist might be influenced by changing the composition of the layered crystals.

The author did the growth of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ single crystal by chemical vapour transport (CVT) technique. The grown single crystals of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ were used for the fabrication of photoelectrochemical (PEC) solar cells. The PEC studies were undertaken in I_2/I electrolytes. The study of varying concentration of electrolytes was studied. The results obtained are deliberated in this research paper.

2. Experimental

2.1 Single Crystals Growth

Stoichiometric amounts of 99.999% pure molybdenum, tellurium and selenium were introduced into a cleaned, etched and vacuum backed quartz ampoule of internal diameter 25 mm and length 200 mm. A total charge of about 9-12 gm was used in the experiment. The transporting agent bromine by weight of $3 \text{ mg} / \text{cm}^3$ to $4 \text{ mg} / \text{cm}^3$ of ampoules volume was introduced into the ampoule in a sealed capillary tube. The ampoule was then evacuated to a pressure less than 10^{-5} torr and sealed at the constriction 3 mm in diameter.

The ampoule was vigorously vibrated to ensure that the capillary tube breaks releasing the bromine and the powders were mixed properly. The mixture was distributed along the length of the ampoule and placed in a two zone horizontal furnace and the temperature was slowly increased to 900°C . The ampoule was left at this temperature for 48 hours.

Then the furnace was shut down and allowed to cool down to room temperature. A free flowing shining dark mixture resulted from the reaction.

The charge thus prepared was well mixed by vigorous shaking of the ampoule. The powder was then placed at one end of the ampoule known as charge zone. Whereas the other end the ampoule was empty for crystal growth to happen and known as growth zone. The ampoule with this distribution of the charge was kept in the furnace again for the growth of crystals as shown fig.1. The furnace temperature was increased slowly, as was done for charge preparation to the required final temperature for growth.

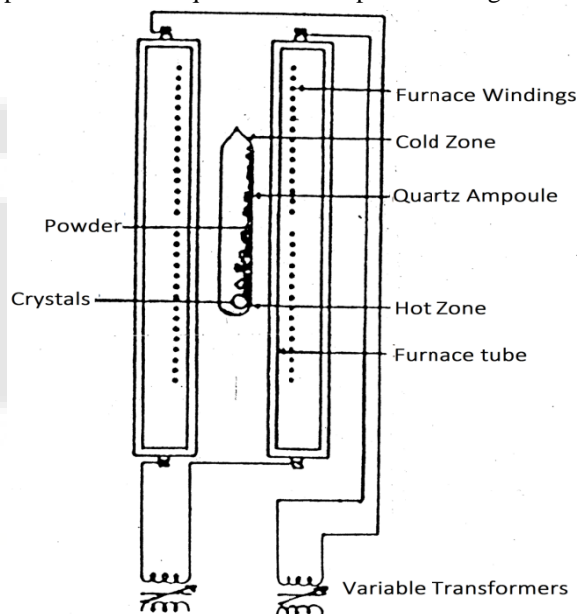


Figure 1: Schematic view of the furnace showing the position of ampoule inside the two furnace during crystal growth.

The exact growth conditions adopted for $\text{MoTe}_{1.5}\text{Se}_{0.5}$ has been described in Table 1. Fig. 2 shows in general the temperature gradient maintained along the ampoule. After the required period of growth the furnace was shut off and allowed to cool down to room temperature. The ampoule was broken and crystals were removed for further studies.

The crystals obtained were grey black, in colour and plate like with the c axis normal to the plane of the plates and all of them grew over the transported charge inside the ampoule.

Table 1: Growth conditions used to produce single crystals of $\text{MoTe}_{1.5}\text{Se}_{0.5}$

Nominal composition	Reaction temperature ($^{\circ}\text{C}$)	Growth temperature ($^{\circ}\text{C}$)	Growth time (hrs)
$\text{MoTe}_{1.5}\text{Se}_{0.5}$	900	800	48

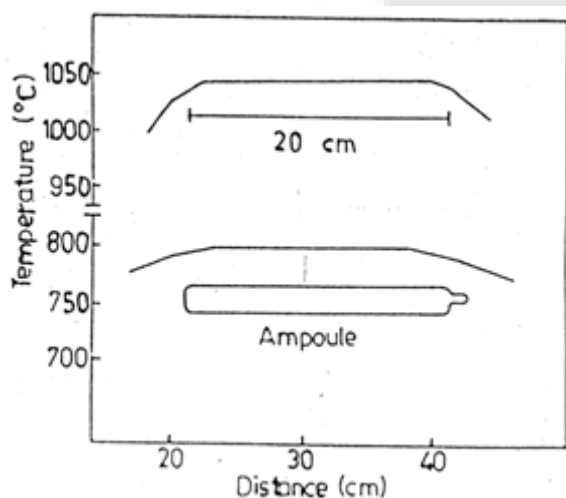


Figure 2: Temperature profile of the furnace

2.2 Photoelectrochemical (PEC) Solar Cells

There have been several discussions in recent years on photoelectrochemical (PEC) methods of solar energy conversion. An important factor affecting the conversion efficiency is the electrolyte. The detailed studies have been carried out by various workers [11-23] on the photoelectrochemical behavior in contact with different aqueous and non aqueous redox electrolytes. Their results have indicated that iodine / iodide, I_2/I^- system to be optimal redox couple for the best performance and stability. Since the light conversion efficiency of the cell based on I_2/I^- depends upon iodine contact of the redox couple, the iodine concentration has been optimized in the present work for better conversion efficiencies of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ photo electrodes.

A key element of PEC devices is the semiconductor electrolyte interface. The degree of effectiveness of minority carrier charge transfer across their interface will have direct bearing on the ultimate energy conversion efficiency of the system.

The strategy of enhancing this charge exchange by electing the temperature has the added advantage of utilizing the near IR region of solar spectrum, which otherwise would be wasted. Temperature also has beneficial effects on the

optical properties of the semi conductor.

An effort has therefore been made to critically evaluate the effect of electrolyte concentration on the photovoltaic performance of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ photoelectrodes.

3. Results and Discussion

Single crystals of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ have been grown by the chemical vapour transport (CVT) technique because it yields large single crystals with relative ease.

The crystals are strain free because they grow vertically in the form of thin platelets directly above the transported charge.

The X-ray diffraction studies of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ indicate that the crystal formed are of single phase.

3.1 Iodine Concentration Effect

The grown single crystals of $\text{MoTe}_{1.5}\text{Se}_{0.5}$ as photo electrodes and platinum grid as counter electrode have been used for fabrication of PEC cells. The photo electrochemical glass cell has been so designed that the electrolyte can be changed without disturbing the electrode position. Electrolytes of different concentrations of iodine are prepared by addition of Na I and Na_2SO_4 in double distilled water. All chemicals are of A.R. Grade. The effect of iodine concentration on the efficiency ($\eta\%$) for $\text{MoTe}_{1.5}\text{Se}_{0.5}$ is shown in figure 3 the decrease in efficiency at higher concentrations of iodine is due to absorption of light in electrolyte which results into lower short circuit currents. The decrease in efficiencies can also be attributed to the presence of large amounts of elemental iodine which can interact with the surface and generate surface states which can trap charges of either sign. This causes large charges of potential drop in Helmholtz double layer as well as shifts in the energy position on band edges. The amount of iodine adsorption, which affects the band bending in the semiconductor, can also be considered as a factor affecting efficiency [19].

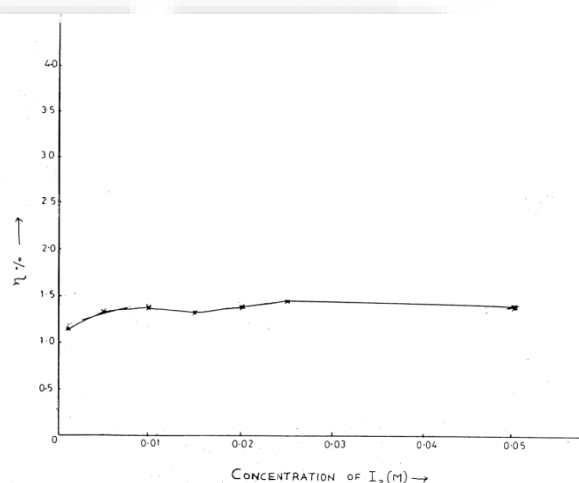


Figure 3: Plot of efficiency versus iodine concentrations $\text{I}_2(\text{M})$ for PEC solar cells based on $\text{MoSe}_{0.5}\text{Te}_{1.5}$

4. Conclusion

The efficiency, fill factor, open circuit voltage and short circuit current of PEC solar cell is found to depend upon the electrolyte content concentration specifically over hereiodine.

5. Acknowledgement

The author is thankful to M.B.Patel Science College, Anand Gujarat, India and the Management of the College for encouraging carrying out the work.

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