Effect Of Temperature Of The Electrolyte On The Performance Of Photoelectro-Chemical (PEC) Solarcells Using Mose$_2$ Single Crystals

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Abstract: The single crystal of $MoSe_2$grown by chemical vapour transport (CVT) technique are used for the fabrication of photoelectrochemical (PEC) solar cells. The effect of the temperature of the electrolyte on the conversion efficiency of the fabricated PEC solar cell is studied.

Keywords: Single crystals, $MoSe_2$, photoelectrochemical solar cell, effect of temperature, 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 $MoSe_xTe_{2-x}(0 \leq x \leq 2)$. Kline et al [8] reported that the transition metal dichalcogenides (TMDCs) forms 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 $MoSe_2$single crystal by chemical vapour transport (CVT) technique. The grown single crystals of $MoSe_2$were used for the fabrication of photoelectrochemical (PEC) solar cells. The PEC studies were undertaken in I_2/I^- electrolytes. The study of varying temperature ofelectrolyte 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 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 mg / cm^3 to 4 mg / 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^{0}C. The ampoule was left at this temperature for 120hours. Then the furnace was shut down and allowed to cool down to room temperature. A free flowing shinning 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 of 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 in fig.1 The furnace temperature was increased slowly, as was done for charge preparation to the required final temperature for growth. The exact growth conditions adopted for$MoSe_2$has been described in Table 1. Fig. 2 shows in general the temperature gradient maintained along theampoule. 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.

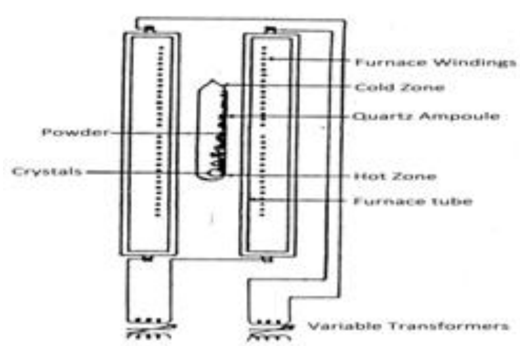

Fig 1: Schematic view of the furnace showing the position of ampoule inside the two zone furnace during crystal growth.

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.

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TABLE 1
GROWTH CONDITIONS USED TO PRODUCE SINGLE CRYSTALS OF $MoSe_2$

Composition	Reaction temperature (^0C)	Growth temperature (^0C)	Growth time (hrs)
$MoSe_2$	900	800	120

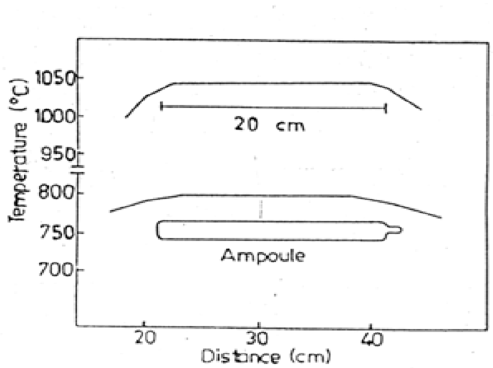

Fig 2: Temperature profile of the furnace.

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-aqueousredox electrolytes. Their results have indicates 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 $MoSe_2$ 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 semiconductor. An effort has therefore been made to critically evaluate the effect of temperature on the photovoltaic performance of $MoSe_2$photoelectrodes.

3. RESULTS AND DISCUSSION

Single crystals of $MoSe_2$have been grown by the chemical vapour transport (CVT) technique because it yields large single crystals with relative ease.The crystals were strain free because they grow vertically in the form of thin platelets directly above the transported charge. The X-ray diffraction studies of $MoSe_2$indicated that the crystalsformed are single phase.

Temperature Effect

The photoelectrochemical solar cell assembly was set up by using $MoSe_2$photoelectrodes and platinum grid as counter electrode. Iodine / Iodide (I_2/I^-) electrolyte was prepared by mixing AR grade 0.025 M I_2,5.0 M NaI, 0.5 M Na_2SO_4 in double distilled water. The temperature of electrolyte was measured by a mercury thermometer. Photocurrent voltage measurements were made at different temperatures, keeping the intensity of illumination constant. An incandescent lamp was used as a source of light. During the heating, electrolyte in the PEC cell was continuously stirred with a magnetic stirrer to maintain an uniform temperature. The effect of temperature on the short circuit current (I_{SC}) and open circuit voltages, at different temperatures is illustrated in figure 3. The open circuit voltages are found to decrease with increase in the temperature. This decreasing trend of Voc is in confirmation with the observation of Kazacoss et al [24].This decrease in open circuit voltage V_{OC} at higher temperature can be explained by applying Schottky barrier model through the equation.

$$V_{OC} = nKT / q \ \ln (I_{ph} / I_o)$$
$$I_0 = A^* T^2 \exp (-\phi_b/KT)$$

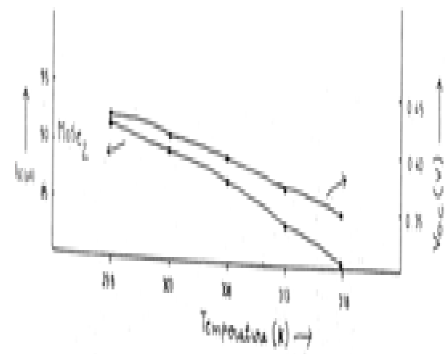

Fig 3: Plots of variations of short-circuit current I_{sc},and open circuit voltage $V_{OC}$of $MoSe_2$based PEC cells with the temperature.

Here A* is Richardson constant and ϕ_b is barrier height. Therefore, according to Schottky barrier model the open circuit voltage V_{OC}, depends upon I_0 the reverse saturation current density, which in turn depends upon the temperature. The initial increase in short circuit current I_{SC} is attributed to the increase in absorption co-efficient of the semiconductor[26]. According to K. Rajewshwaret. al.[27] the increase in short circuit current I_{SC} has its origin both on temperature induced changes in the optical and electrical properties of semiconductor and corresponding variations in the potential and charge distribution across the semiconductor electrolyte interface. It is observed by Agarwal et.al.[28] that

1. The wavelength response shifts towards red with increasing temperature because of band gap narrowing.
2. The diffusion length of photogenerated carriers increases with increasing temperature, and
3. The absorption coefficient at longer wavelength increases with increasing temperature because of band gap narrowing.

All this jointly causes increase in I_{SC} with increasing temperature. The increase in I_{SC} is however limited because of changes in series and shunt resistances of the cell with temperature. At higher temperature, shunt resistance decreases reducing the current in the cell. The bulk resistance of semiconductor also decreases with increasing temperature. The observed peak of current (I_{ph}) is a result of these two competing factors. At still higher temperatures shunt resistance of the cell becomes smaller and the current decreases further. From fig. 3 the short circuit current I_{SC} for$MoSe_2$is found to increase with increase in temperature. Similar trends in short circuit current is also observed by Kazacoss et al [24]. Figure 4 illustrates the variation of the efficiency and fill factors of $MoSe_2$ PEC cells at different temperatures. The efficiency of the cells shows a maximum value at 308K while the fill factor increases with the increase in temperatureand shows a maximum value at 318 K. Similar trends of efficiency and fill factor is also observed for $MoSe_2$based PEC solar Cell [14].

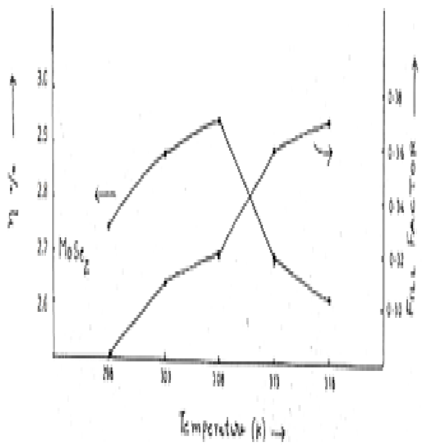

Fig 4: Plots of variations of conversion efficiency (η%) and fill factor of MoSe2 based PEC cells with the temperature.

TABLE 2.
JUNCTION IDEALITY FACTOR FOR $MoSe_2$

Compound	Ideality factor calculated 'n'
$MoSe_2$	2.0

CONCLUSION

1. The efficiency, fill factor, open circuit voltage and short circuit current of PEC cell is found to depend upon operating temperatureof the solar cell.
2. The open circuit voltages shows a decreasing trend in their values with the increase in temperature
3. Peak in efficiency is found at about 308 K.

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