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PEC solar cell behaviour of $NbSe_2$ and NbS_2 single crystals grown by DVT technique

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Abstract

Transition Metal dichalcogenides constitute a well- defined family of compounds which crystallize in a layer type structure. These compounds have energy band gap close to the solar spectrum maxima and hence they form an important class of solar cell materials. P-N junction and other solid junction solar cells are practical form of solar cells which have been, by now, transformed from research level to commercial shape; where as solid – liquid junction solar cells have some limitations for their commercialisation. Nevertheless, they form an important tool to study electrochemical interaction for characterizing different material properties of semiconductor electrode. In this paper authors have attempted to fabricate Photoelectrochemical solar cell with semiconductor electrode using crystals of NbX_2 (X= S, Se) grown by Vapour transport techniquei. E. Direct Vaapour Transport (DVT) technique. Two solar cell electrodes using single crystals of $NbSe_2$ and NbS_2 as photoelectrodes have been prepared. A mixture of iodine [I_2], potassium ferricyanide [$K_3Fe(CN)_6$] and potassium ferrocyanide [$K_4Fe(CN)_6$] was employed as an electrolyte with concentration of 0.025M I_2 + 0.1M [$K_4Fe(CN)_6$] + 0.1M [$K_3Fe(CN)_6$]. The dark and polychromatic solar cell responses were recorded with the help of incandescent lamp varying intensity of illumination between 30 mW/cm^2 to 120 mW/cm^2. The solar cell parameters like fill factor (FF), Open circuit Voltage (V_{oc}), Short circuit Current (I_{sc}) and photoconversion efficiency (η) for both the cells have been determined. The obtained results are discussed in reference to the intensity and wavelength of incident radiation.

Keywords: PEC solar cells, Crystal Growth, Fill factor and photo conversion efficiency.

Introduction

Transition metal dichalcogenides (TMDCs) have attracted considerable attention for fabricating the Photo electrochemical (PEC) solar cell electrode[1]. The reason is that available in both, n-and p-type nature, have energy band gaps in solar absorption maxima and well suited to solar energy conversion, a high absorption coefficient in the visible range, an extremely good stability and no effect of corrosion when they are in contact with various aqueous and non-aqueous electrolytes and they are cheap and abundant. Metal chalcogenides such as GeS, GeSe etc. are technologically important class of group IV-VI materials. They possess layered structure which are bonded by weak Van der Wall's bonding. Due to this layered structure they exhibit large anisotropy in physical, chemical and electronic properties which are explored to realize applications such as solid state lubricant, solar cell, EFT, phase change memory etc. devices. Recently after invention of graphene, there has been an upsurge in the research activities pertaining to monolayer studies of these materials. Exotic property changes and related devices are a subject matter of these materials today as they undergo a transition from indirect to direct band gap material on transforming them from bulk to monolayer form. Different structural, chemical compositional, electrical, thermoelectric properties are proposed to be studied in order to know the suitability of grown materials for their application and use in some junction based semiconductor devices like Photo electrochemical Solar Cells (PEC). Apart from this on application of pressure this class of materials undergo a structural phase change and hence effect of pressure on electrical properties of this materials are also proposed to be studied in this work.

Materials and methods

Crystal growth: In the present investigations $NbSe_2$ and NbS_2 crystals have been grown by Vapor transport technique I.e. Direct vapour Transport (DVT) technique. Dual zone horizontal furnace having required dimensions has been used for placing quartz ampoule as shown in Figure-1. The furnace was constructed by a special sillimanite threaded tube closed at one end, 450 mm in length, 70 mm outer diameter, 56 mm inner diameter with threaded pitch of 3 mm, imported form from Koppers Fabriken Feuerfester, Germany. Very High quality quartz ampoules were used for crystal growth experiment. These quartz ampoules have dimensions of 24 cm length, 2.4 cm outer diameter and 2.2 cm inner diameter. For compound preparation the ultra-cleaned quartz ampoule was filled with stoichiometric proportion of Nb (99.999%), S (99.99%) and Se (99.99 %) pure of about 10 g for growth. Ampoule was sealed under pressure of 10^{-5}Torr so that there is no effect of air molecules and surrounding gases. The sealed ampoule was kept in dual-zone horizontal furnace as shown in the Figure-1[2]. The temperatures of the two zones i.e. source zone and growth zone were slowly but gradually raised up to desired temperature at 20 K/hr keeping some temperature gradient of 50 K and maintained that temperature for 80 hours. The temperature of the furnace was lowered at the rate of 20 K/hr upto the room temperature (i.e. 300K). The quartz ampoule was broken and fine crystals were taken out and used as photoelectrode. These growth parameters with crystals dimensions are mentioned in Table-1.

Table-1: Growth conditions for $NbSe_2$ and NbS_2 crystals.

Compositions	Temperature (K)		Growth Period (hours)	Crystal Dimensions (mm × mm)
	Source zone	Growth zone		
$NbSe_2$	1173	1123	80	15 ×8
NbS_2	1173	1123	80	16 × 8

Preparation of semiconductor electrode: Crystals with plane faces i.e. crystals with step free surfaces were employed after a careful examination of the samples under an optical microscope. Step free van der Walls surfaces could be easily obtained from the grown crystal by cleaving the as grown samples with an adhesive tape. A glass rod of 0.5 cm in diameter and 10 to 12 cm in length with a narrow bore of diameter 0.05 cm was used to prepare the electrode. One end of this narrow bore glass rod was flattened by hot gas blow to make a circular platform such it the flat portion could be used as a platform for resting the crystal[3]. The narrow bore was used as a passage for traversing a good conducting copper wire. The copper wire was flattened at one end for getting a contact with the crystal[4].

Counter electrode: A counter electrode in PEC solar cells is required to complete the electrochemical reactions in a cell for better performance of PEC solar cell. Generally Platinum or Copper is widely used material for the same[5].

Selection of appropriate electrolyte: The selection of appropriate electrolyte in a PEC solar cell is extremely important because it actually is a source for the electrochemical reactions leading to the photo-effects. The electrolyte consists of the oxidized and reduced species. These species should be ionic in nature, which help in transfer of photo generated carrier from the photo-electrode to the counter electrode. To obtain a necessary photo conversion efficiency from Photo electro chemical solar cell, the selection of appropriate electrolyte plays a vital role in energy conversion. The electrolyte decides the efficiency of photo conversion. Here we have used 0.025M I_2 + 0.1M $[K_4Fe(CN)_6]$ + 0.1M $[K_3Fe(CN)_6]$ as an electrolyte[5].

Experiment setup of photo electrotchemical solar cell for I-V characteristics: The semiconductor electrode prepared in the manner outlined above was dipped in an appropriate electrolyte contained in a glass beaker. Copper grid (2cmX2cm) played the role of the counter electrode. A schematic diagram of the photo electrochemical solar cell is shown in Figure-3. Illumination of the cell was provided with different light intensity from a tungsten filament bulb (incandescent lamp). The illumination intensity I_L was changed by changing the distance between the electrode and the bulb. The incident intensity of illumination was measured using solar meter (LUX meter). Biasing Voltage was applied across the electrodes and corresponding Photocurrent was recorded using Keithley 2400 multimeter operated using LAB TRACER software. The I-V characteristics of PEC solar cell in ideal cases as well as in practical cases is shown in Figure-4. The I-V characteristics of practical cases largely deviate from ideal characteristics[6].

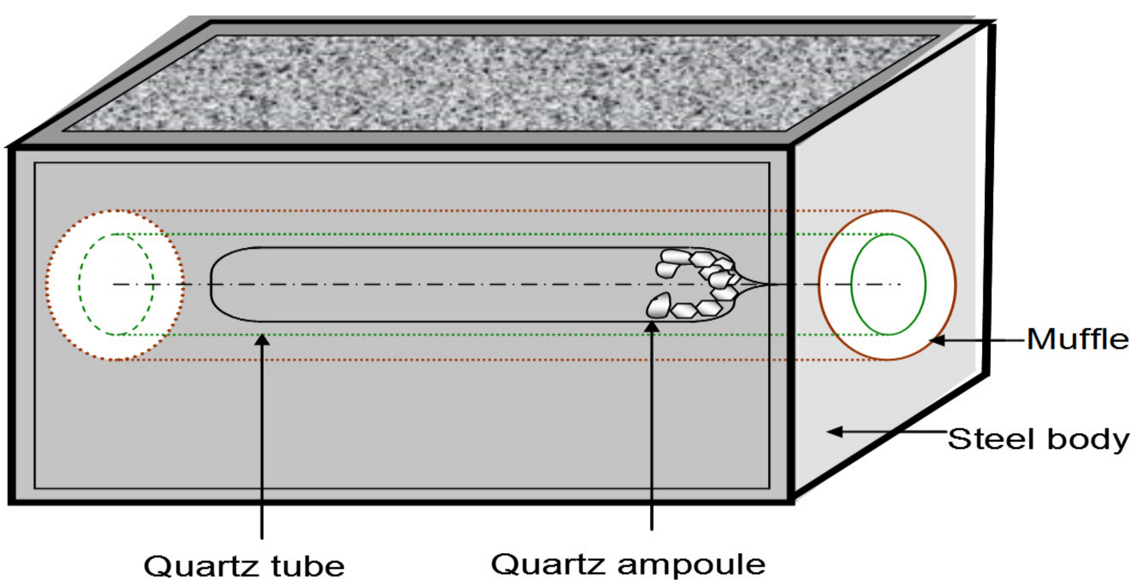

Figure 1: Dual zone horizontal furnace with co-axially loaded ampoule[14].

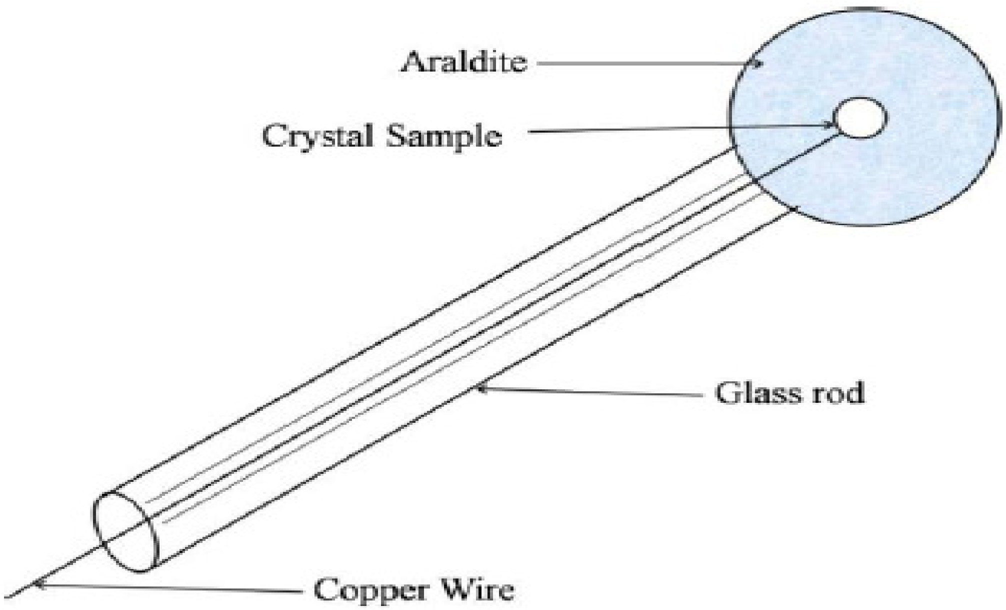

Figure-2: Semiconductor electrode for PEC solar cell[14].

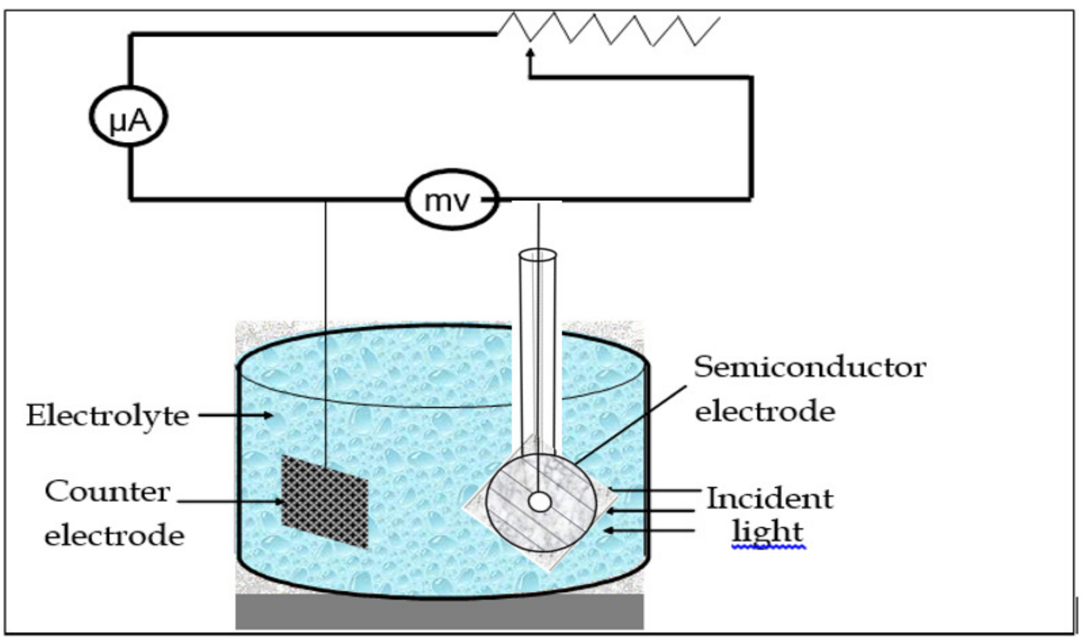

Figure-3: The schematic diagram of PEC solar cell used to measure I-V characteristic.

Electrode: $NbSe_2$ and NbS_2 single crystal. **Area of Crystal:** 0.004cm^2($NbSe_2$) 0.017cm^2(NbS_2). **Electrolyte:** 0.025M I_2 + 0.1M [$K_4Fe(CN)_6$] + 0.1M [$K_3Fe(CN)_6$] **Counter Electrode:** Copper.

Photoelectrochemical solar cell using single crystals of NbX_2 (X= S, Se) as a semiconductor electrode grown by direct vapour transport (DVT) technique. Two solar cell electrodes using single crystals of $NbSe_2$ and NbS_2 as photoelectrodes have been prepared[7]. A mixture of iodine [I_2], potassium ferricyanide [$K_3Fe(CN)_6$], potassium ferrocyanide [$K_4Fe(CN)_6$] was employed as an electrolyte with concentration of 0.025M I_2 + 0.1M [$K_4Fe(CN)_6$] + 0.1M [$K_3Fe(CN)_6$]. The dark and polychromatic solar cell responses were recorded with the help of incandescent lamp varying intensity of illumination between 30 mW/cm^2 to 120 mW/cm^2. The solar cell characteristic output parameters like Short Circuit Current (I_{sc}), Open Circuit Voltage (V_{oc}), Fill Factor (FF) and photo conversion efficiency (η) for both the cells have been determined. The obtained results are discussed in reference to the intensity and wavelength of incident radiation[8].

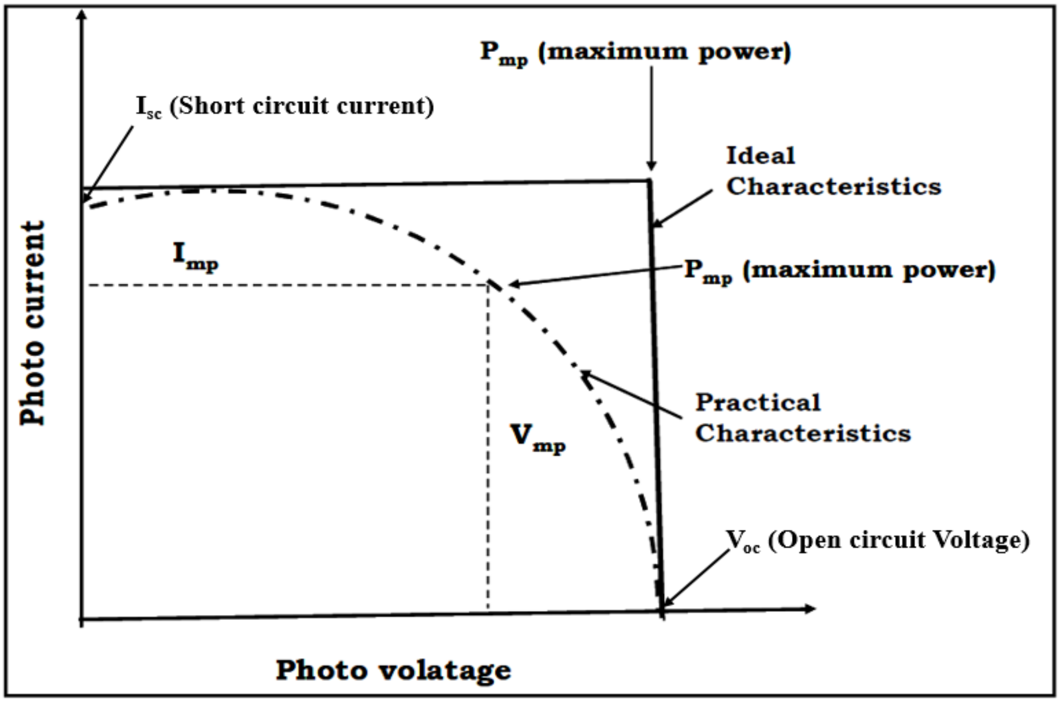

Figure-4: Ideal and Practical I-V characteristic of solar cell.

Characteristic parameters of PEC solar cell: *Short circuit current (Isc):*

$$I_{sc} = I_o\left[\exp\left(\frac{eVoc}{kT} - 1\right)\right]$$

Where: I_0= Reverse saturation current. *k* = Boltzmann constant. T = Operating temperature (Room temperature). V_{oc}= Open circuit voltage.

Open circuit voltage (Voc):

$$V_{oc} = \left(\frac{nkT}{e}\right)\ln I_L$$

Where: n = ideality factor. kT/e = 0.0259 volt at 300K. I_L = Intensity of illumination.

Fill Factor (FF):

$$F.F = \frac{J_{mp} \times V_{mp}}{J_{sc} \times V_{0c}}$$

Where: J_{sc} is the short circuit current density, J_{mp} is the current density at maximum power point, V_{mp} is the voltage at maximum power point.

Photo conversion Efficiency (η%):

$$\eta = \frac{V_{mp} \times I_{mp}}{P_{in}} = \frac{F.F \times V_{oc} \times I_{sc}}{P_{in}} \times 100\%$$

Quantum efficiency (nq):

$$\mathbf{n_q} = \frac{\text{Number of photogenerated electrons/ unit area}}{\text{Number of incident photons/ unit area}}$$

Results and discussion

An amalgamation of $K_3\,[Fe(CN)_6]$,$K_4\,[Fe(CN)_6]$and I_2 was used as an electrolyte. Electrolyte solutions were prepared using double distilled water[9].

It was observed that electrolyte with the composition 0.025M I_2 + 0.1M $[K_4Fe(CN)_6]$ + 0.1M $[K_3Fe(CN)_6]$ gave the maximum value of photocurrent and photo voltage for all the electrodes and minimum dark voltage V_D and dark current I_D well suited to be used as electrodes. So it was used as an electrolyte[10].

The Open circuit Voltage (V_{oc}) and Short circuit Current (I_{sc}) show a large deviation from the linear dependence on the intensity of incident illumination with reference to the ideal case[11].

V_{oc} and I_{sc} show a small deviation for polychromatic and monochromatic sources of different intensities.

The large deviation in I-V characteristics from ideal behaviour is due to the fact that there are several other parameters associated with materials, electrolyte, incident light, incident light intensity and the semiconductor-liquid electrolyte interface which governs the effective photo generation and charge transfer mechanism[12].

The area under the I-V characteristics increases with increase in the intensity of incident illuminations[13] as shown in Figure-5 and 6.

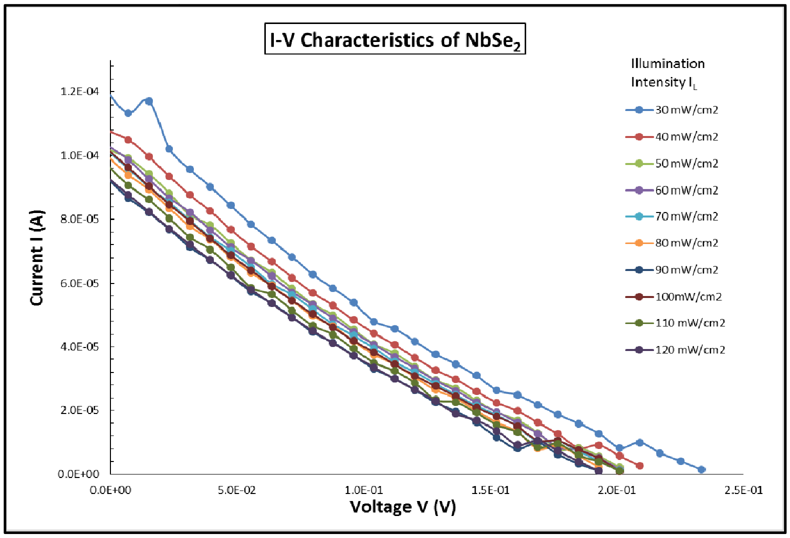

Figure-5: I-V Characteristics of $NbSe_2$ single crystal.

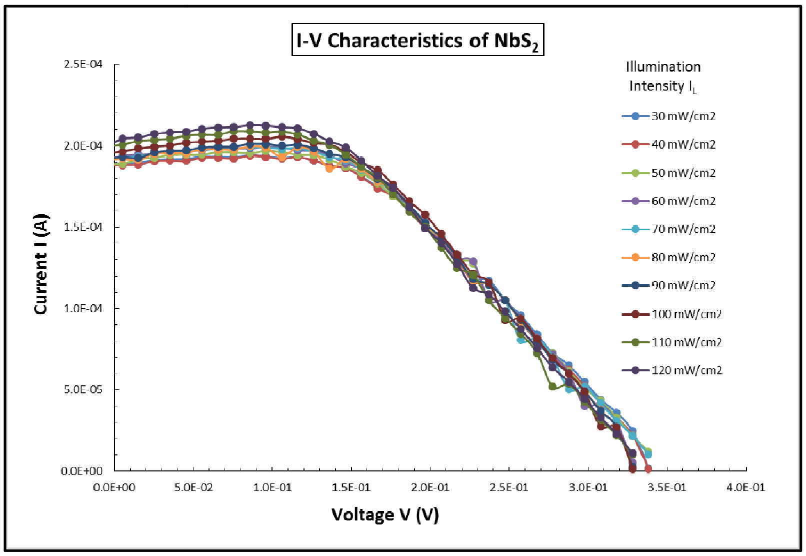

Figure-6: I-V Characteristics of NbS_2 single crystal.

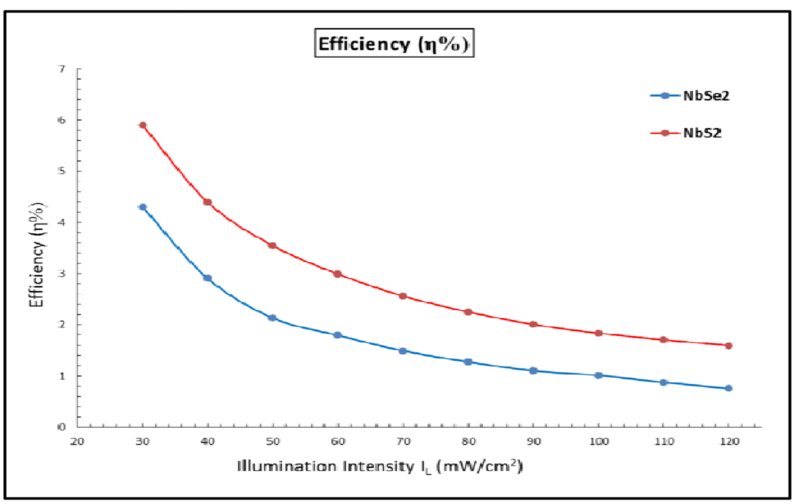

Figure-7: Efficiency comparison between $NbSe_2$ and NbS_2 single crystal.

Table-2: Parameters of the investigated PEC solar cell.

Illumination Intensity mW/cm2	I_{sc}(A)		V_{oc} (V)		Fill Factor		Efficiency (η%)	
	$NbSe_2$	NbS_2	$NbSe_2$	NbS_2	$NbSe_2$	NbS_2	$NbSe_2$	NbS_2
30	1.2E-04	1.9E-04	2.3E-01	3.4E-01	0.19	0.47	4.30	5.90
40	1.1E-04	1.9E-04	2.1E-01	3.4E-01	0.21	0.47	2.91	4.39
50	1.0E-04	1.9E-04	2.0E-01	3.4E-01	0.21	0.47	2.13	3.54
60	1.0E-04	1.9E-04	2.0E-01	3.3E-01	0.21	0.49	1.79	2.99
70	1.0E-04	1.9E-04	2.0E-01	3.4E-01	0.21	0.52	1.49	2.56
80	1.0E-04	1.9E-04	1.9E-01	3.3E-01	0.21	0.49	1.27	2.25
90	9.8E-05	1.9E-04	2.0E-01	3.3E-01	0.20	0.49	1.10	2.00
100	1.0E-04	2.0E-04	2.0E-01	3.3E-01	0.20	0.49	1.01	1.83
110	9.7E-05	2.0E-04	2.0E-01	3.4E-01	0.20	0.47	0.88	1.70
120	9.3E-05	2.0E-04	1.9E-01	3.4E-01	0.20	0.48	0.75	1.59

Conclusion

Single crystal of $NbSe_2$ and NbS_2 semiconductor were successfully grown using Vapour Transport technique i.e. Direct Vapour Transport (DVT) technique. We have synthesized this crystal used this crystal as an electrode in photo electrochemical solar cell and interpreted the variation of solar cell characteristic output parameters like Open circuit Voltage V_{oc}, Short circuit Current I_{sc}, Fill Factor and Efficiency η% (Figure-7) vary little but they are directly dependent on the Illumination intensity I_L of polychromatic light as shown in the Table-2.

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