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# Current transport mechanisms studied by I-V-T measurement on Cu-$n$MoSe$_2$ Schottky diode

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Cu-nMoSe$_2$ Schottky diode has been fabricated and the current transport mechanism of the prepared diodes have been investigated for a temperature range of 320K-50K. From the I-V results various Schottky barrier parameters were evaluated. It has been observed that the ideality factor increases with decrease in temperature and its value increases from: 1.1 at 320K to 67.3 at 50K. On the other hand, the barrier height decreases with decrease in temperature and its value at 320K is 0.72eV which becomes 0.1eV at 50K.

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## 1. Introduction

There has been a growing interest in the use of layered molybdenum diselenide crystals (MoSe$_2$) being its flexible nature along with good carrier mobility [1-3]. This make them potential candidate for fabricating flexible high mobility electronic devices such as Schottky barrier devices, FETs, solar cell etc [4-7]. These devices will rely on a rectifying metal-semiconductor contact for its operation. Therefore the study of current transport mechanism with suitable metal contacts to MoSe$_2$ is of great interest. The performance and reliability of such Schottky diode is drastically influenced by the interface quality between the deposited metal and the semiconductor surface. In this paper, we have investigated the characteristics of Schottky contacts using thermally evaporated copper as a basic metal for studying n-MoSe$_2$ for a temperature range of 320K-50K.

There are different methods for measurement of Schottky barrier height and related parameters. They are; (i) photoelectric method, (ii) current-voltage method, (iii) Activation energy method, (iv) conductance-voltage method, (v) capacitance-voltage method and (vi) photoelectron spectroscopy method. The most widely used amongst these are current-voltage, activation energy and photoelectric measurement methods. As far as small contacts are concerned, as in the case of contacts used in deep submicron technology, the use of activation energy and photoelectric method is not suitable due to area restriction. Thus current-voltage measurement method is found suitable to extract barrier parameters by its analysis. Besides this, it shows the nature of rectification property of contacts under test. Therefore in present investigations current-voltage measurement method is used for evaluation of barrier parameters. Therefore, with the help of I-V as the measurement technique, various Schottky barrier parameters were calculated by the following methods. They are: [8 -10]

**1.** V versus ln I method
**2.** V versus ln{I/[l-exp(-qV/kT)]} method

The plot of V vs ln I yield a straight line for $V > \left(\frac{3kT}{q}\right)$ and this may cover two to three decades of change in current at low forward bias voltages. The intercept on y-axis of this straight line gives the value of saturation current $I_0$. From this $\Phi_{b0}$ can be calculated using equation,

$$\Phi_{b0} = \frac{kT}{q}\ln\left(\frac{AA^{*}T^{2}}{I_0}\right) \quad (1)$$

Also from the slope of the V vs ln I plot, the ideality factor n can be calculated as,

$$n = \frac{q}{kT}\frac{dV}{d(\ln I)} = \frac{q}{kT}\times\frac{1}{slope} \quad (2)$$

The more realistic representation of barrier potential is done if the bands are flat across the interface. Under this condition the barrier potential as designated by flat band barrier height is given by [11]

$$\Phi_{bf} = n\Phi_{bo} - (n-1)\frac{kT}{q}\ln\left[\frac{N_C}{N_D}\right] \quad (3)$$

Here $N_D$ is the carrier concentration of MoSe$_2$. The value of $N_D$ is found to be of the order of $10^{15}$cm$^{-3}$ from Hall effect measurement. $N_C$ is the effective density of state in the conduction band, which is given by [9],

$$N_C = 2\left[\frac{\left(2\pi m_e^* kT\right)}{h^2}\right]^{3/2} \quad (4)$$

where, $m_e^*$ is the effective mass of $MoSe_2$ and is given by $0.5m_0$ [12]. Here $m_0$ is the rest mass of electron ($9.1x10^{-31}$ kg), k is boltzmanns constant ($1.3808 \times 10^{-23}$ J/K or $8.6175 \times 10^{-5}$ eV ), T is the temperature in K and h is planks constant. Using these values $N_C$ comes out to be $8.84 \times 10^{24}(m^{-3})$.

The analysis with V vs ln I plots give reliable values of barrier parameters if:

**(i)** it is a straight line covering two to three decades of current change and

**(ii)** it should fit to several low forward voltage observation points. But in many practical devices this plot is neither a straight line because of large series resistance or it covers much observed values of V and I. Thus a *V* versus ln{I/[l-exp(-qV/kT)]} plot is made at each temperature mainly to cover the wide bias range including the regime $V < \left(\frac{3kT}{q}\right)$ where the 1 - exp(- qV/kT) factor is effective. The straight line portion of such a plot corresponds to the thermionic emission diffusion current with the intercept giving saturation current $I_0$. The slope of this line gives the ideality factor *(n)* according to the following equation,

$$n = \frac{q}{kT} \times \frac{1}{slope} = \frac{q}{kT} \frac{dV}{d\ln\left[\frac{I}{1-\exp\left(\frac{-qV}{kT}\right)}\right]} \quad (5)$$

and $\Phi_{b0}$ using equation 1.

In order to study the charge transport mechanism in the $MoSe_2$ based Schottky diodes number of diodes were prepared and analyzed. The subsequent section presents the analysis of one such typical diode.

## 2. Experimental procedure

Initially the direct vapour transport (DVT) grown crystals of $MoSe_2$ with flat shining surfaces, chosen with the help of optical microscope, were washed in acetone to remove contaminations and to make the surface clean; and later they were dried in the oven at $60^0$C. The cleaned crystals were mounted on the substrate holder inside the vacuum chamber.

In this study metal dots were deposited using thermal evaporation technique. In order to get evaporated metals on a confined area on the crystal surface, crystals were masked with a thin metal sheet having fine circular holes. After reaching a vacuum level, pure copper metal was evaporated (3kÅ) from a W-helical boat onto the semiconductor surface. The rate of evaporation was kept very slow i.e.2Å/sec in order to make the deposition uniform over the whole area. In addition, this definitely gives good adhesion and other desirable properties in the Schottky diode fabrication by relatively slower growth mechanisms.

Front Schottky contacts with evaporated copper regions were taken with low strain copper wires and Au paste (Eltec-1228C). The back (ohmic) contacts were taken with indium metal ingot which was fused onto the surface of $MoSe_2$ along with low strain thin Ag alloy wires with the help of a fine tip of soldering iron. The whole assembly was fixed on a mica piece for support and utmost care was taken during the whole process to keep the prepared structure intact because $MoSe_2$ crystals are very much soft and brittle. This was then mounted on the sample mount stage inside the Closed Cycle Refrigerator (CCR 75014) and contacts were soldered.

Since current – voltage (I-V) analysis is the basic and simplest of all methods due to direct measurement of current and voltage and provides first hand information about the nature of the developed barriers across the interface, the analysis were done with the help of I-V method. I-V data were acquired using Keithley – semiconductor Characterization System SCS-4200. The variation of current and voltage with temperature were accomplished by liquid helium close cycle refrigerator controlled by Lakeshore temperature controller. The experiment was repeated at different temperatures from room temperature to cryogenic temperature of around 20K in steps of 10K.

## 3. Experimental results and discussion

The total current passing through a Schottky barrier device may be because of one or a combination of several conduction mechanisms. The general understanding of dominant charge transport mechanism can be done by the comparison of the magnitude of energy characteristics $E_{00}$ with that of kT/q. The value of $E_{00}$ can be calculated from the equation 3. Since $N_D$ is a temperature dependent parameter the value of $E_{00}$ calculated for different temperature regions. Result shows that in these temperature ranges $\frac{kT}{E_{00}} >> 1$ [14] and TE conduction mechanism has been identified as the dominant charge transport mechanism.

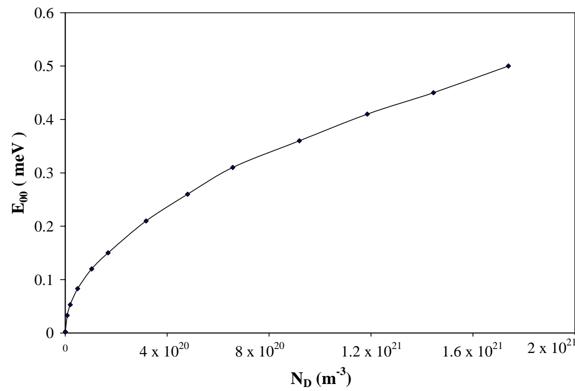


*Fig. 1. Variation of $E_{00}$ as a function of change in $N_D$ observed at different temperatures.*

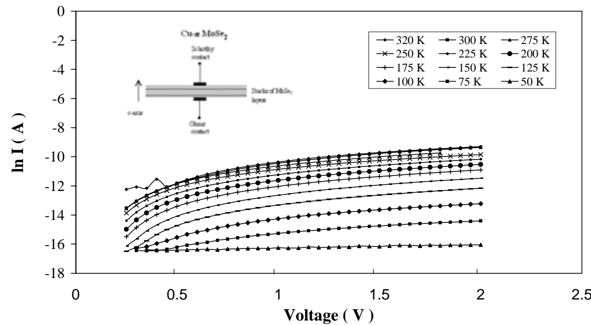


*Fig. 2. shows the semi-log I-V characteristics of Cu-nMoSe$_2$ Schottky diode measured at various temperatures ranging from 300-50K.*

The slops of the linear portions of these curves were calculated and the ideality factors were determined using the relation 2 for temperature ranging from 50K-320K. The intercept on y – axis of semi-log plot of current voltage curve was used to determine the value of saturation current ($I_S$) and using this value the barrier heights were calculated for the range of temperatures. The dependence of barrier height and ideality factor on temperature is shown in figure 3. It has been observed that the ideality factor increases with decrease in temperature and its value increases from: 1.1 at 320K to 67.3 at 50K. On the other hand, the barrier height decreases with decrease in temperature and its value at 320K is 0.72eV which becomes 0.1eV at 50K. Various factors may be responsible for these large variations observed in ideality factor and barrier height. The ideality factor is simply a manifestation of the barrier uniformity and it increases for an inhomogeneous barrier [15]. An apparent increase in ideality factor and decrease in BH at low temperature are possibly caused by some other effects such as inhomogeneities of thickness and composition of the layer, non-uniformity of the interfacial charges or the presence of any thin insulating layer between the metal and the semiconductor [16 -21].

Since the current transport across the MS interface is a temperature-activated process, at low temperature, the current will be dominated by the current through the patches of low barrier height. Therefore at low temperature, electrons are able to overcome the lower barriers, and hence current transport will be dominated by current flowing through the patches of lower BH and resulting in to larger ideality factor. As the temperature increases, more and more electrons have sufficient energy to overcome the higher barriers. As a result both BH and n are strongly dependent on temperature. Moreover, simulation studies of Freeouf *et al* [22] on mixed-phase Schottky contact reveal that, below a critical size, low BH region pinched off and high barrier remains effective

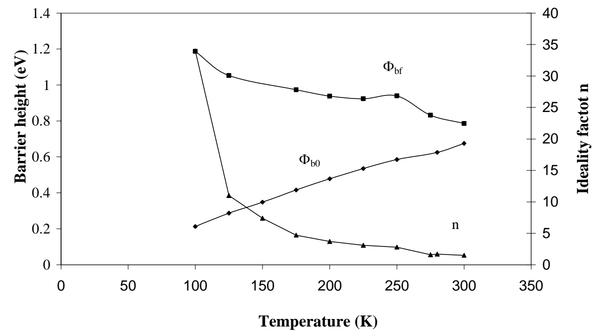


*Fig.3. Plot of ideality factor, zero-bias barrier height and flat band barrier height as a function of temperature for he Cu-nMoSe$_2$ Schottky diode.*

Schmitsdorf *et al* [23, 24] used Tung's theoretical approach and they found a linear correlation between the experimental zero-bias BH and ideality factors n. Figure 4 show a plot of the experimental SBH as a function of the ideality factors dependent on temperature. As can be seen from the figure there is nearly linear relationship between the experimentally observed effective BHs and ideality factors of Cu-*n*MoSe$_2$ SBDs that is explained by lateral inhomogeneities of the BHs in the SBDs [25, 26]. From the plot one can see that the ideality factor n =1 has a homogeneous BH of 0.78 by extrapolating the plot. The other barrier height values are deviating from this value due to local inhomogeneities. In order to obtain the flat-band barrier height the analysis of Wanger *et al* and chin has been followed. The flat-band barrier height is calculated from the equation 3 mentioned earlier. The temperature dependent $N_C$ and $N_D$ values are used in calculating $\Phi_{bf}$ values. The variation of flat band barrier height at various temperature ranges is shown in figure 5. From the data it can be seen that the flat-band barrier height is invariably larger than the zero-bias barrier height at low temperatures. This is possibly due to extremely high values of the ideality factor, which increases with decreasing temperature. In contrast to the case the zero-bias BH, the electric field in the semiconductor is zero under flat-band conditions and thus the effect of tunneling and image force lowering that would affect the I-V

characteristics and removes the influence of lateral inhomogeneity.

The temperature dependence of the $\Phi_{bf}$ is expressed as $\Phi_{bf} = \Phi_{bf}(T = o) + \alpha T$, where $\Phi_{bf}(T = o)$ is the barrier height extrapolated to zero temperature and $\alpha$ is the temperature coefficient of the barrier height. The fit of above equation to the data as shown in figures5 gives $\alpha = -1.9 \times 10^{-3} eV / K$ with $\Phi_{bf}(T = o)$ as 1.33eV.

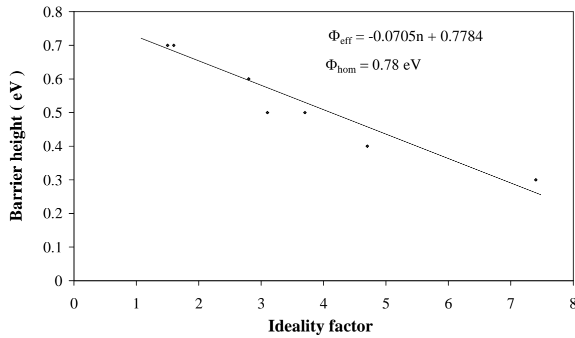


*Fig. 4. The variation in zero-bias barrier height versus ideality factor.*

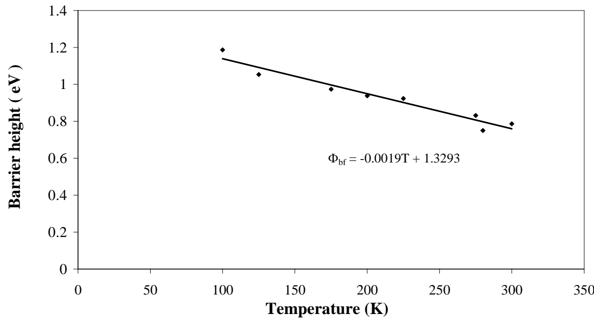


*Fig. 5. The temperature dependence of flat-band barrier height.*

The Richardson plot of $\ln I_0/T^2$ vs 1000/T is drawn to obtain the barrier height in another way. From thermionic emission theory we can rewrite,

$$\ln\left(\frac{I_0}{T^2}\right) = \ln\left(AA^*\right) - \frac{q\Phi_{b0}}{kT} \quad (6)$$

The saturation current $I_0$ is found from the intercept of the straight lines from the semi-log plot of I-V curve with the ordinate. Fig. 6 shows the $\ln\left(\frac{I_0}{T^2}\right)$ versus $\left(\frac{1000}{T}\right)$ curve. According to equation 6 the curve yields a straight line with a slope given by the barrier height at 0 K and the intercept given by the Richardson constant.

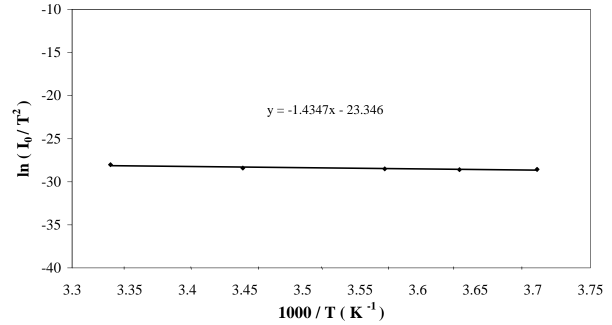


*Fig.6. Richardson plot of ($\ln I_o/T^2$) versus $10^3/T$ for the Cu-nMoSe$_2$ Schottky diode.*

The value of $A^*$ obtained from the intercept of the straight portion at the ordinate is equal to 23.3 Acm$^{-2}$ K$^{-2}$. This value is lower than the calculated value 59. But the value of $\Phi_{bf}(T = o)$ is very much comparable with the one obtained from the flat-barrier height.

## 4. Conclusions

Cu-$n$MoSe$_2$ Schottky diode has been fabricated and tested for a temperature range of 300K – 50K. The current voltage characteristics of the fabricated diode shows good rectification ratio. Also it could be seen that the representative forward current characteristics do not exhibit exponential rise with voltage and reverse I-V characteristics do not show saturating nature. This represents non-ideal nature for both forward and reverse bias conditions. Thus it can be expected that the characterizing parameters of fabricated diodes might be associated with both bias dependent and temperature dependent natures arising from various physical reasons.

The charge conduction mechanism in this diode has been found to be thermionic emission (TE) from the temperature dependent values of donor density and the tunneling parameter $E_{00}$. On the basis of this, various Schottky diode parameters were deduced. The decrease of barrier height with decreasing of temperature may be attributed to the interface states, inhomogeneous nature of the fabricated diode, multiple transport mechanisms involved in the conduction of carriers etc.

The ideality factor calculated for the same temperature range of 300K-50K shows that as temperature decreases the ideality factor increases. The inhomogeneous thickness and composition of the layer, non-uniformity of the interfacial charges, the presence of any thin insulating layer between the metal and the semiconductor etc. may ascribed for the change of barrier height and ideality factor at low temperatures.

From the linear relationships of barrier height and ideality factor a homogeneous barrier height of 0.78 has

been found. The other barrier height values are deviating from this value due to local inhomogeneities. The flat-band barrier height calculated at various temperatures show that its value is much larger than the zero-bias barrier height at low temperatures. This may be due to the high value of ideality factor at low temperatures. Also from the temperature dependent flat-band barrier the value of temperature coefficient of the barrier height has been deduced. The value is found to be $-1.9 \times 10^{-3}$ eV/K. The flat band barrier height at zero Kelvin is found to be 1.33eV. The Richardson plot drawn for the given diode yields a straight line by giving the Richardson constant as $23.3 \text{Acm}^{-2}\text{K}^{-2}$ and $23.7 \text{Acm}^{-2}\text{K}^{-2}$ respectively for both the geometries.

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