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Simulation of Perovskite channel Thin Film Transistor

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Abstract

A bottom gate thin film transistor has been simulated and analyzed in which the channel is made up of lead perovskite ($CH_3NH_3PbI_3$) using Silvaco Atlas software. The perovskite channel thin film transistor shows high field effect mobility and transconductance which makes the transistor very attractive for display devices applications. The field effect mobility of perovskite channel thin film transistor obtained through simulations matches closely with the experimentally reported field effect mobility. The transistor has been modified by adding a metal layer to the gate which significantly enhances the transconductance of the perovskite channel thin film transistor. The same transistor has been simulated by using tin perovskite ($CH_3NH_3SnI_3$) instead of lead perovskite ($CH_3NH_3PbI_3$) as channel material to avoid harmful effects associated with the presence of lead in lead perovskite. The tin perovskite channel thin film transistor also exhibits high performance parameters which makes the transistor a potentially suitable environment friendly device for modern electronic applications.

Keywords: Perovskite, Thin film transistor, Field effect mobility.

I. INTRODUCTION:

In last decade there has been huge rise in the use of mobile phones, laptops and flat panel display TV's. This has led to an extraordinary rise in the demand of display devices in the market. There is an ever-increasing competition among companies to produce better and cheaper displays. Thin Film Transistor (TFT) is one of the basic component of these display devices. Display devices are used in displays of mobiles and laptops which occupy large area. Therefore, these thin film transistors should also be of low cost otherwise the cost of displays would become prohibitively large. Therefore, low cost amorphous silicon is commonly used in the fabrication of thin film transistors instead of costly crystalline silicon and amorphous silicon based display devices have found widespread use for last many years. But low mobilities of amorphous silicon thin film transistors puts major limitation on the performance of display devices. Also, in the recent years there has been an increasing trend to make the devices like mobile phones with mechanically flexible displays. Such flexible displays use plastic substrate instead of conventional silicon substrate. Therefore, thin film transistors of flexible displays must also be compatible with such plastic substrate. This requires that the thin film transistors should also have low temperature processability otherwise it will damage the plastic substrate. To meet this requirement organic semiconductor based thin film transistors have been developed in the last few decades [1]. The first organic semiconductor based thin film transistor was reported in 1989 [2]. Since then organic semiconductor based thin film transistors have seen huge progress and now possess advantages like low temperature solution processability, mechanical flexibility along with low cost fabrication [3-4]. Due to these advantages organic thin film transistors have been successfully used in various applications like displays, radio frequency identification (RFID) and sensors [5-10].

Although organic thin film transistors offer many advantages as mentioned above but they have a major drawback. The mobility of organic thin film transistors has been so far mostly restricted to the order of 1 $cm^2/V\text{-}s$ [11]. Due to this organic thin film transistors are not suitable for many applications which require high switching speeds. Hence there is a need for thin film transistor which may exhibit high mobility and also have low cost and low temperature fabrication process.

In the recent years, organic-inorganic perovskite materials have been found to possess such set of properties which can potentially be used to make high quality thin film transistors. These perovskite materials especially organolead metal halide perovskites have attracted huge interest of the research community which is reflected by the large number of research publications in this area in the last decade. They combine the advantages of both organic and inorganic materials. They show excellent optical properties, high mobilities, long diffusion lengths along with the low cost and low temperature fabrication techniques [12-15]. In fact, due to these properties of perovskite materials, photovoltaic technology has seen significant improvement in the last few years. Therefore, it can also be expected that the perovskite material will perform better than amorphous silicon and organic semiconductors in thin film transistor applications. Such perovskite based thin film transistors can potentially operate at high switching speeds like inorganic transistors and at the same time combine advantages of organic transistors like low temperature and low cost processibility and mechanical flexibility. Although extensive work has been done on photovoltaic applications of perovskite materials but still there is lack of sufficient work on the perovskite based thin film transistors [16-19]. There are few reports of fabrication of perovskite based thin film transistors in the recent years [20-22]. The field is still in its initial phase of development and hence there is massive scope of research and development in perovskite based thin film transistors. The goal is to have a perovskite based thin film transistor with high mobility and transconductance along with low cost processing so that it can work on high switching speeds of modern circuits. Apart from experimental research, device simulation has proved to be an effective tool in the development of electronic devices as it helps to reduce the cost and time. Simulations can help to gain insights which may not be possible otherwise in many cases. Moreover, currently there is lack of work in the field of simulation of perovskite based thin film transistors. Hence in this work we have simulated a bottom gate thin film transistor in which the channel is made up of perovskite thin film. In these simulations firstly we have used methyl ammonium lead iodide ($CH_3NH_3PbI_3$) as channel in the transistor and secondly tin perovskite ($CH_3NH_3SnI_3$) has been used as the channel material. Tin perovskite has been used as $CH_3NH_3PbI_3$ contains lead which is toxic and thus harmful for environment. Lead poisoning can cause serious damage to humans and can even be fatal. Performance parameters of the thin film transistors have been extracted which shows the efficacy of perovskite thin film transistors. Transistor structure has also been modified to improve the performance. The results show that the perovskite channel transistor can be an exciting choice for many modern applications. As presently there are no simulation study of perovskite thin film transistor, so it is hoped that this work would help to motivate further work in this interesting field.

II. DEVICE STRUCTURE AND SIMULATION PARAMETERS:

Thin film transistor (TFT) is a field effect transistor in which the conducting channel is made by an accumulation layer which differs from the case of conventional silicon based metal-oxide-semiconductor field effect transistors (MOSFET) where the conducting channel is made by an inversion layer. Fig. 1 shows the device structure of the perovskite channel thin film transistor. It has the structure of a bottom gate thin film transistor where the gate is at the bottom side and the source and drain terminals are at the top. In this thin film transistor the channel is made up of lead perovskite having the chemical formula, $CH_3NH_3PbI_3$. $CH_3NH_3PbI_3$ is an ambipolar material (both electron and hole have same value of mobility). The perovskite channel has been taken as n-type with the doping concentration of 10^{16} cm^{-3}. The device has a thin film of perovskite deposited over a thin film of silicon dioxide. The substrate of the device has not been shown in Fig. 1. The thickness of both perovskite film and oxide film has been taken as 200 nm. The width (W) and of the thin film transistor is 5 mm and the length (L) of the channel is 500 µm. All contacts (source, drain and gate) are made of aluminium. The material parameters of the device have been carefully selected from the literature and are listed in Table I [23-25]. The fabrication of such type of thin film transistor has been reported by Yuxiang et al [25]. Width (W) and channel length (L) of our transistor have been taken equal to those of the thin film transistor reported by Yuxiang et al. Silvaco Atlas software has been used for all the simulations of thin film transistor in this work.

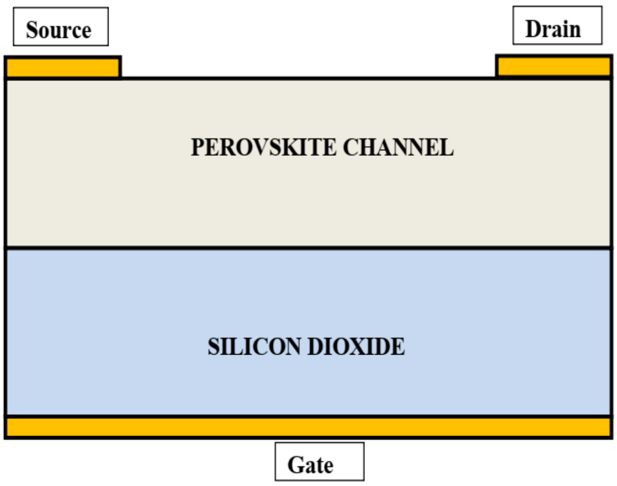

Fig 1. Device structure of perovskite channel thin film transistor.

Table I. Material parameters of perovskite $CH_3NH_3PbI_3$.

Perovskite Parameters	Values
Bandgap Eg	**1.55 eV**
Relative Permittivity	**6.5**
Electron Affinity	**3.75 eV**
Electron mobility	**400 cm^2/V-s**
Hole mobility	**400 cm^2/V-s**
Conduction band density of states Nc	**2.2×10^{15} cm^{-3}**
Valence band density of states Nv	**2.2×10^{17} cm^{-3}**
Donor Density N_D	**10^{16} cm^{-3}**

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III. RESULTS AND DISCUSSIONS:

The perovskite channel thin film transistor has been simulated to plot the drain current (I_D) versus the gate to source voltage (V_{GS}) graph. Drain to source voltage (V_{DS}) has been fixed at 2 V. Fig. 2. shows the device structure which is obtained through ATLAS simulations. Fig. 3. shows the variation of drain current as V_{GS} is varied from -20 V to 20 V. The transconductance of thin film transistor g_m has been calculated from the I_D- V_{GS} curve (Fig. 3.) using the equation:

$$gm = \frac{\partial ID}{\partial VGS} \qquad -(1)$$

This gives us the transconductance, gm = 1.425×10^{-4} S. Fig. 4 shows the family of I_D- V_{DS} curves corresponding to different values of V_{GS} which resembles typical n channel TFT characteristic curve.

The field effect mobility, μ_{FE} of the thin film transistor has been calculated using the following equation:

$$\mu_{FE} = \frac{Lgmtox}{\varepsilon oxWVDS} \qquad -(2)$$

where W and L are the width and channel length of thin film transistor, oxide thickness (tox) = 200 nm, relative permittivity of oxide= 3.7. Using above equation, for V_{DS} = 2V, the field effect mobility (μ_{FE}) of thin film transistor is found to be equal to 435.18 cm^2/V-sec. This value is close to the experimentally reported value of 396.2 cm^2/V-sec [25]. This is also close to the mobility values of perovskite taken by us in the simulations initially (400 cm^2/V-sec as shown in Table I). This validates our simulation to a large extent.

Similarly, threshold voltage and On Current to Off Current ratio (I_{ON}/I_{OFF}) have been extracted from the I_D-V_{GS} curve and are found to be:

$$V_T = -0.51 \text{ V}$$

$$I_{ON}/I_{OFF} = 1.85\times10^{10}$$

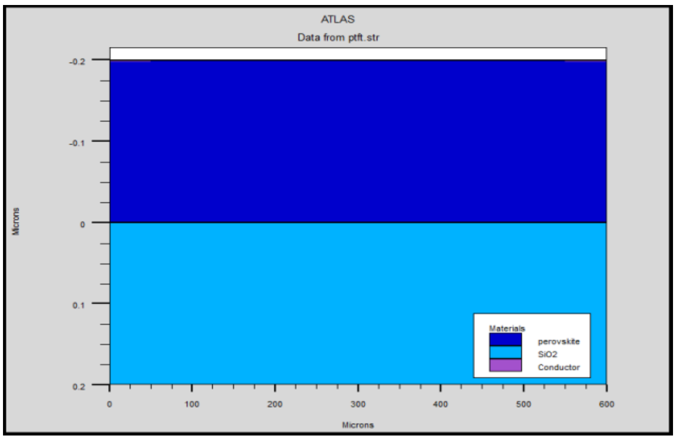

Fig. 2. Device structure obtained from ATLAS simulator.

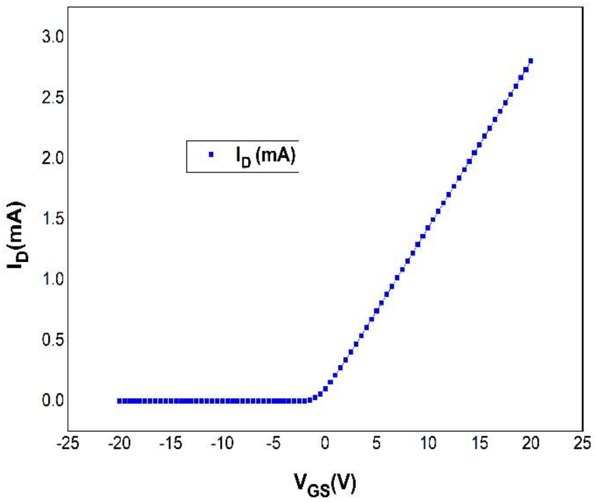

Fig. 3. I_D- V_{GS} curve of perovskite channel thin film transistor.

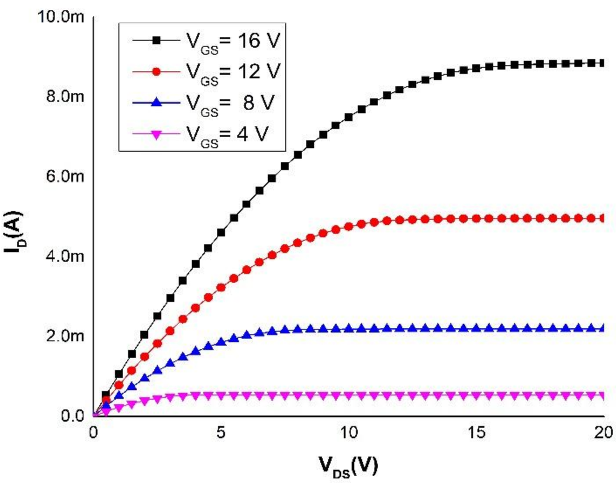

Fig. 4. I_D- V_{DS} curve of perovskite channel thin film transistor.

As can be seen from the above performance parameters of the device it can be said that the perovskite channel thin film transistor exhibits field effect mobility performance similar to some inorganic transistors. This comes along with the added advantages of low temperature processing. It can be said that it combines the advantages of both organic and inorganic semiconductor-based transistors. This makes the device very attractive for display devices applications.

In order to improve the performance of this device we have added one additional layer of aluminium on top of perovskite film between source and drain terminals as shown in Fig. 5. This aluminium layer is connected to the gate of the transistor on the bottom side. We call this a modified perovskite thin film transistor (modified PTFT). The addition of this metal layer is expected to increase the control of gate over the channel.

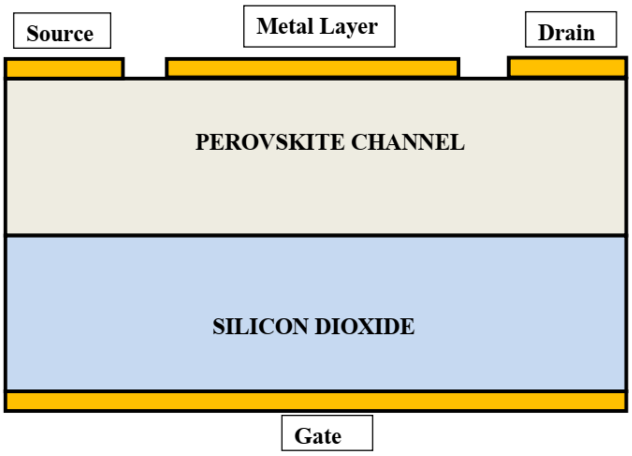

Fig. 5. Modified perovskite channel thin film transistor.

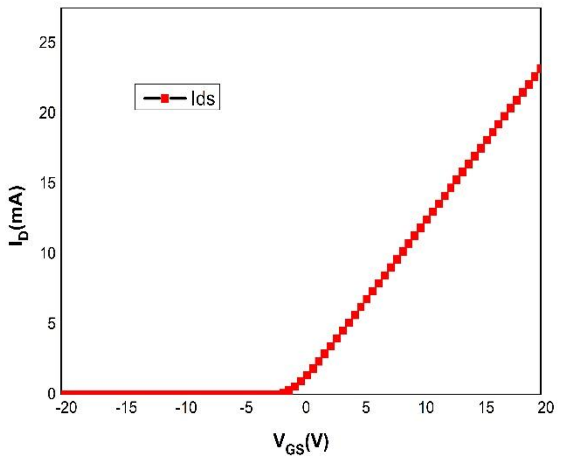

Fig. 6. I_D- V_{GS} curve of modified perovskite channel thin film transistor.

The modified thin film transistor has been simulated for V_{DS} = 2V and the corresponding I_D- V_{GS} curve has been shown in Fig. 6. From the I_D- V_{GS} curve transconductance has been calculated using eq (1) and is found to be:

$$gm = 1.5\times10^{-3}\ S$$

Threshold voltage V_T has been calculated by linear extrapolation of I_D-V_{GS} curve of Fig. 6. and is found to be:

$$V_T = -0.51\ V$$

I_{ON}/I_{OFF} ratio has also been extracted from I_D-V_{GS} curve and is found to be:

$$I_{ON}/I_{OFF} = 1.11\times10^{11}$$

The performance parameters of both the perovskite channel thin film transistors (PTFT) have been compared in Table II. It is observed that the threshold voltage of both the transistors are same. It can also be seen that the transconductance and I_{ON}/I_{OFF} ratio of modified perovskite channel thin film transistor is larger than that of the original thin film transistor. This happens because after addition of metal layer on top of perovskite channel, the gate affects the channel from both top and bottom side of channel. This increases the control of gate over the channel and transconductance is actually a measure of the control of channel through the gate. Hence the transconductance of transistor also increases in the case of modified structure. Similarly, the increase in the transconductance increases the on current (I_{ON}) which increases the I_{ON}/I_{OFF} ratio of modified PTFT. Thus, it can be said that the modified PTFT has overall better performance than the original PTFT.

Table II: Comparison of parameters:

Parameters	**PTFT**	**Modified PTFT**
g_m	**1.425×10^{-4} S**	**1.5×10^{-3} S**
V_T	**-0.51 V**	**-0.51 V**
I_{ON}/I_{OFF}	**1.85×10^{10}**	**1.11×10^{11}**

The above analysis shows that the perovskite channel thin film transistors have huge potential for wide variety of applications. These transistors show much better mobilities than the mobilities of amorphous silicon based thin film transistors commonly used in modern display devices. Perovskite based solar cells have already shown much better performance than silicon based solar cells and count among the best solar cells presently.

But there is one major issue with the thin film transistor analyzed here. The channel of the thin film transistor is made of $CH_3NH_3PbI_3$ which contains lead. Lead is a toxic element and has harmful effects on human health. This puts restriction on the use of lead perovskite devices. Hence there have been efforts to find lead free perovskite materials to replace lead perovskite in various applications. Tin perovskite has been found to be the suitable perovskite to replace lead perovskites in photovoltaic applications and many tin perovskite solar cells have been reported in the literature [26-27]. Tin perovskite films with very low trap density and large diffusion lengths have been reported in literature [24]. Therefore, here we select tin perovskite as channel material for thin film transistor to investigate its performance. Rest of the device parameters are same as the parameters of single gate $CH_3NH_3PbI_3$ channel thin film transistor analyzed earlier in this paper. The material parameters of tin perovskite channel used in the simulations have been selected from the literature and are listed in Table III [28-30]. Tin perovskite has been taken as p-type material as Sn^{2+} gets easily oxidised into Sn^{4+} through self-doping process in films of $CH_3NH_3SnI_3$ [31] .

Tin perovskite thin film transistor has been simulated for V_{DS}= 2V. The corresponding I_D-V_{GS} curve of tin perovskite channel thin film transistor is shown in Fig. 7. Thus, transconductance and field effect mobility of tin perovskite TFT have been found to be [as extracted from I_D-V_{GS} curve (Fig. 7) by using equation (1) and (2)]:

gm = 5.38×10^{-6} S.

μ_{FE} = 16.04 cm^2/V-sec.

V_T = 1.5 V

$I_{ON}/I_{OFF} = 1.86 \times 10^{11}$

These values of performance parameters show that tin perovskite thin film transistors can be good choice for large number of electronic applications. Finally we have done the comparison of field effect mobilities of various types of thin film transistors in Table IV. It can be seen from the Table IV that the field effect mobility of lead perovskite thin film transistor is highest. It is also higher than the field effect mobility of polysilicon TFT's. Field effect mobility of tin perovskite channel thin film transistor is smaller than the field effect mobility of $CH_3NH_3PbI_3$ channel thin film transistor. But still it is higher than the mobility of amorphous silicon and organic semiconductor based thin film transistors. Also it is not toxic like lead perovskite devices.

Table III. Material parameters of tin perovskite ($CH_3NH_3SnI_3$).

Perovskite Parameters	**Values**
Bandgap Eg	**1.3 eV**
Relative Permittivity	**8.2**
Electron Affinity	**4.17 eV**
Electron mobility	**1.6 cm^2/V-s**
Hole mobility	**1.6 cm^2/V-s**
Conduction band density of states Nc	**10^{18} cm^{-3}**
Valence band density of states Nv	**10^{18} cm^{-3}**
Acceptor Density N_A	**10^{15} cm^{-3}**

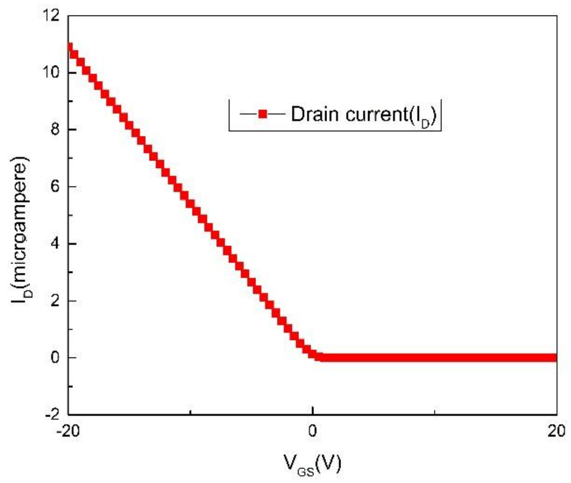

Fig. 7. I_D-V_{GS} of Tin perovskite thin film transistor.

Hence this also shows that the $CH_3NH_3SnI_3$ channel thin film transistor can possibly be a suitable choice to replace amorphous silicon thin film transistors in display devices. But presently there are very few reports of fabrication of perovskite thin film transistors in the literature. This is the first simulation study of perovskite thin film transistor to the best of our knowledge. Also there are no reports of $CH_3NH_3SnI_3$ channel based thin film transistors to the best of our knowledge. This work shows the exciting potential of such perovskite channel thin film transistors for various applications. They have potential to replace costly inorganic transistors in variety of applications. But lot of research work is required in this field to move perovskite thin film transistors into commercial domain. It is hoped that this work will motivate further research work in the field of perovskite transistors.

Table IV: Comparison of field effect mobilities:

S. No.	Thin film transistor (TFT) type	Field effect mobility (cm^2 /V-sec)	Reference
1.	Lead Perovskite TFT	435.18	This work
2.	Tin Perovskite TFT	16.04	This work
3.	Amorphous Silicon TFT	0.3	[32]
4.	Polysiicon TFT	100	[33]
5.	Organic TFT	3.6	[34]

IV. CONCLUSION:

Lead perovskite ($CH_3NH_3PbI_3$) channel bottom-gate thin film transistor has been analyzed with the help of simulations using Silvaco Atlas software. The transistor shows high field effect mobility, transconductance and I_{ON}/I_{OFF} ratio. The field effect mobility obtained through simulations matches closely with the experimentally reported field effect mobility of perovskite channel thin film transistor which validates the simulation model. To improve the performance of perovskite channel thin film transistor the device structure has been modified which increases the transconductance of transistor. Tin perovskite channel thin film transistor has also been investigated which can avoid the lead toxicity associated with lead perovskite transistor. It shows lower field effect mobility than the field effect mobility of lead perovskite channel thin film transistor but still significantly higher than those of amorphous silicon thin film transistors commonly used in display devices. These results show that perovskite channel thin film transistors can potentially replace inorganic thin film transistors in display devices applications and hence more efforts should be devoted in this relatively unexplored area.

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