

STUDY TO FIND OUT IF IT POSSIBLE TO HAVE A TANDEM SOLAR USING THE  
STRUCTURE Si/SRO/TCO

Index

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## 1. Analysis of a MIS capacitor for application in solar cells

### i. Introduction

The solar cell call "STIMULATED INVERSION LAYER SOLAR CELL (SIL)" is made of a Transparent Conductive Oxide (TCO), silicon rich oxide and silicon, and it has three possibilities of generate electrical energy from Sun light. The first one is through an inversion layer produced by charging the SRO. This concept has been proved experimentally. The second one takes advantage of the nanocrystals produced in the solar cell, there are some papers that shows that photovoltaics effects are observed in SRO [1, 2, 3] [4]. The third possibility is if we can use the TCO as a semiconductor and add the energy generated by this layer to that of the silicon solar cell. This will be equivalent to a tandem solar cell. There are many reports that uses TCO to form semiconductor-insulator-semiconductor (SIS) heterojunction solar cells. So, for this analysis it is assumed that TCO, and in particular the Zinc Oxide doped with Aluminum (AZO), behave as a semiconductor, in the same way that silicon does. AZO is the TCO used for this analysis, but any other that complains with the requisites of transparency and electric conductivity can be used.

The objective of this analysis is to find out the conditions in which both semiconductors AZO and silicon are in the depletion regimen, in such a way that in they both the charge separation take place. The Zinc Oxide band gap has been reported in the literature as 3.3 eV and the affinity 4.5 eV [5], and it is N type. So, it is adequate to propose that in AZO the ZnO band gap is constant, and the Fermi level varies with the Al doping. A big variation of the fermi level has been also reported for AZO [4, 5, 6 and 7], so in this analysis we suppose that the Fermi varies under the conduction band.

Another detail not addressed here is how the electron pairs generated in the silicon and that in the AZO can be added to increase the efficiency of the system.

### ii. Assumptions

1. Both Silicon and AZO are considered semiconductor.

2. AZO first is considered degenerated, or as a Metal, and it is not affected by the work functions difference or the charge in the Oxide. Then, a variation on the Fermi level is considered, and then a band bending is taken in consideration.

### iii. Surface potential

To find out the silicon surface potential, we assume that:

1. Both Silicon and AZO are considered semiconductor.
2. AZO first is considered degenerated, or as a Metal, and it is not affected by the work functions or the charge in the Oxide. Then, a variation on the Fermi level is considered, and then a band bending is taken in consideration.
3. The dielectric is a perfect insulator, and it has not any charge.
4. The band ideal diagram of the system is show in figure 1.
5. The AZO band gap is 3.3 eV and that of Silicon is 1.1 eV
6. Because, we work only with magnitudes the units are volts.
7. For calculation we use an N type silicon with  $1 \times 10^{14} \text{ cm}^{-3}$  density of donors.

#### a) Silicon surface regime when AZO is as a metal

Table 1 shows different characteristics of the silicon when the AZO is supposed that behave as a metal and the work function is the same as the electron affinity.

Silicon threshold voltage were calculated for different concentrations as show in table 1.

As can be observed in figure 1, ideally when there is not any effect on the band diagram of both TCO and silicon, the band diagrams are misaligned. However, in equilibrium the fermi levels in AZO and in silicon are aligned, to do so the silicon band has to move down as shown in figure 2. As seen in figure 2, The silicon band bending is such that its surface has to be in depletion regime or in inversion.

To find out if the silicon surface is in depletion or in inversion, the silicon surface potential ( $\Psi_s$ ) will be found.

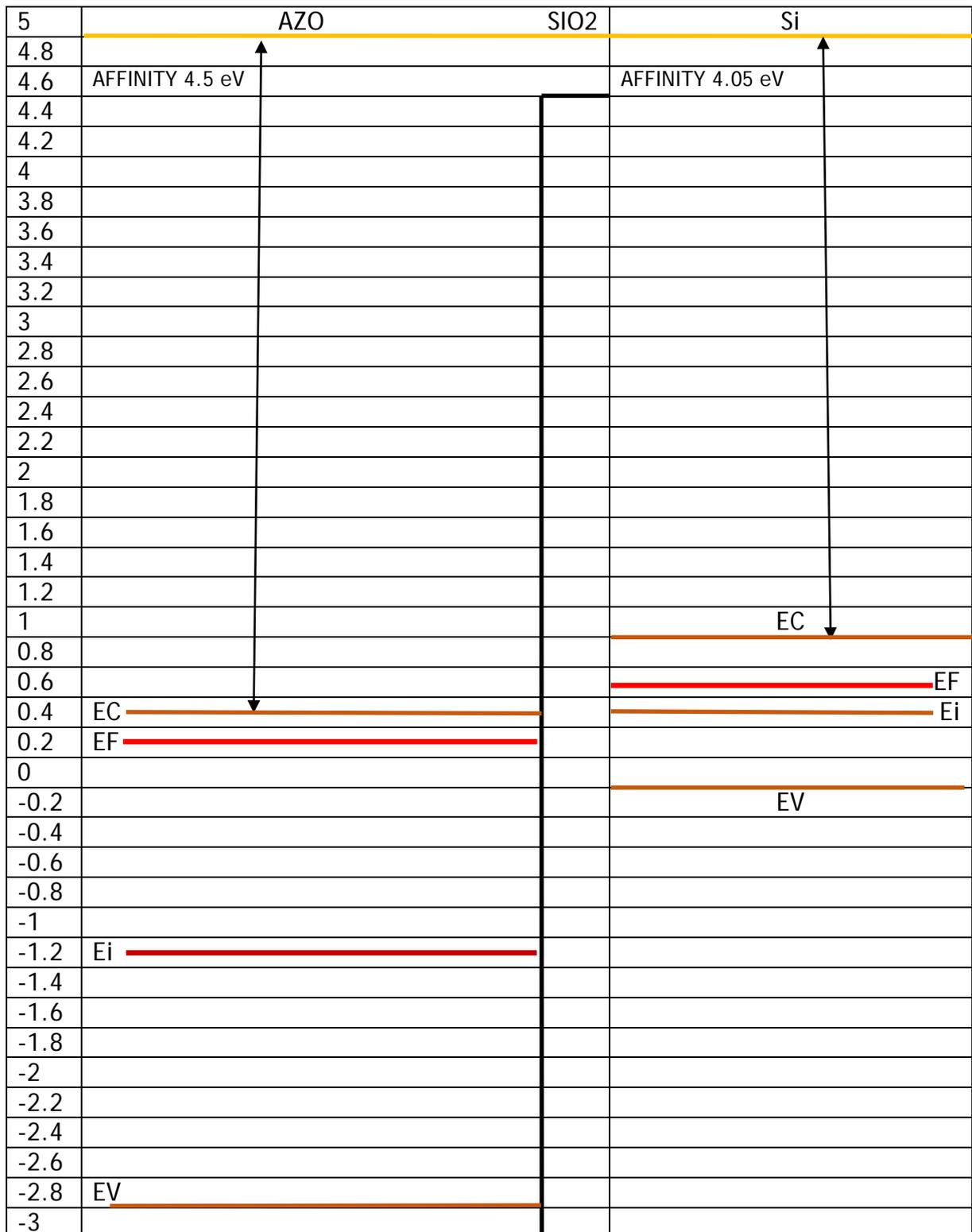


Figure 1. AZO/SiO<sub>2</sub>/Si ideal band diagram the electron affinity of both materials are shown. The n type Si band gap is approximated 1.1 eV, N<sub>D</sub> is 10<sup>14</sup> cm<sup>-3</sup>, the Fermi level is approximated to 0.33 eV under the conduction band. The AZO is N type and the band gap is approximated to 3.3 eV. For clarity, the AZO conduction band and the Fermi level were separated.

Table1. density of donors ( $N_D$ ), bulk potential ( $\Psi_B$ ), Fermi level ( $E_f$ ), Work function ( $\phi_s$ ), AZO-silicon work function difference ( $\phi_{As}$ ), the magnitude of the threshold voltage ( $V_t$ ), the AZO work function in this case is the same as the AZO Affinity ( $X$ ) and equal to 4.5 V

$N_D \text{ cm}^{-3}$	$\Psi_B \text{ V}$	$F_f \text{ V}$	$\phi_s \text{ V}$	$\phi_{As} \text{ V}$	$V_t \text{ V}$
1.00E+12	0.11	0.44	4.49	0.005	0.24
1.00E+13	0.17	0.39	4.44	0.065	0.37
1.00E+14	0.23	0.33	4.38	0.125	0.68
1.00E+15	0.29	0.27	4.32	0.185	1.63
1.00E+16	0.35	0.21	4.26	0.245	4.75
1.00E+17	0.41	0.15	4.20	0.304	15.23
1.00E+18	0.47	0.09	4.14	0.364	50.40
1.00E+19	0.53	0.03	4.08	0.424	167.93

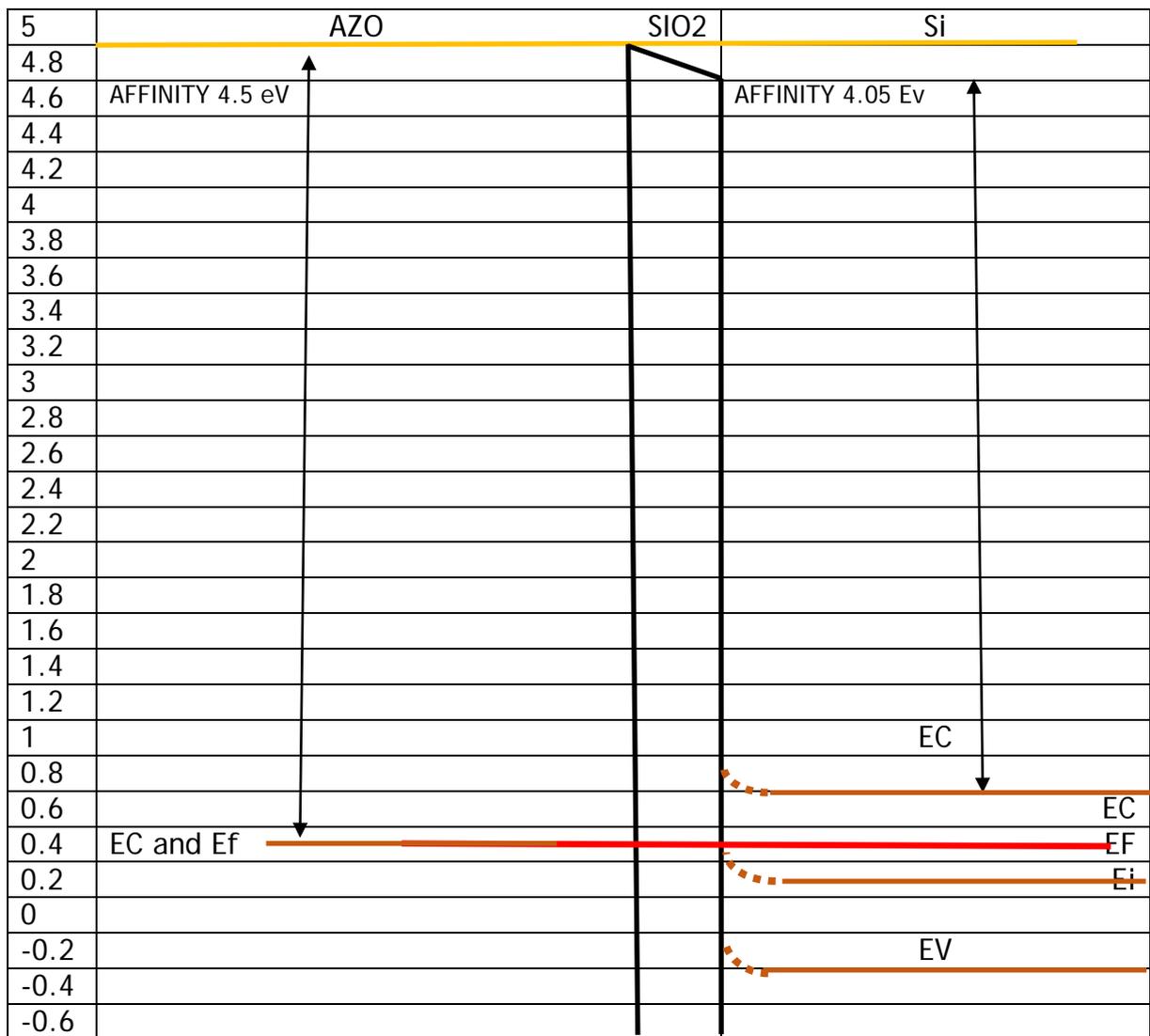


Figure 2. Silicon band bending, the band bending indicates the silicon Surface is in depletion or inversion. For the sake of clarity, it is supposed that the vacuum level and the silicon oxide conduction band is the same.

From table 1, it is observed that for all the silicon doping concentration the  $V_t$  is always bigger than the work function differences, so we can say that the silicon surface is in depletion. The following mathematical analysis will confirm this asseveration.

The only cause of the band bending is the difference in work functions. Then,

$$\varphi_{As} = \frac{Q_E}{C_{ox}} + \Psi_s = V_{ox} + \Psi_s \quad V. \quad (1)$$

$\Psi_s$  is the silicon surface potential,  $Q_E$  is the charge in the silicon surface and  $C_{ox}$  is the oxide capacitance,

$$Q_E = qN_B W. \quad (2)$$

$W$  is the depletion width and  $N_B$  is the bulk doping density, and

$$C_{ox} = \frac{\varepsilon_{ox}}{t_{ox}} \quad (3)$$

$C_{ox}$  is the oxide capacitance, where  $\varepsilon_{ox}$  is the dielectric constant, and  $t_{ox}$  is the insulator thickness.

From the definition of depletion charge, equation (1) can be written as:

$$\sqrt{\frac{2\varepsilon_s}{qN_B}} \psi_s = (-\psi_s + \varphi_{As}) \frac{C_{ox}}{qN_B} \quad (4)$$

and from here we obtain the quadratic equation (5)

$$0 = \beta \psi_s^2 - (2\beta \varphi_{As} + 1) \psi_s + \beta \varphi_{As}^2. \quad (5)$$

Here

$$\beta = \left( \frac{C_{ox}^2}{2q\varepsilon_s N_B} \right) = \frac{(\varepsilon_{ox}/t_{ox})^2}{2q\varepsilon_s N_B}, \quad (6)$$

and

$\epsilon_{ox} = 0.33 \times 10^{-12} \frac{F}{cm}$  is the oxide dielectric constant,

$t_{ox} = 300 \times 10^{-7} cm$ , is the oxide thickness,

$q = 1.6 \times 10^{-19} coul$  is the electronic charge,

$N_B = 1 \times 10^{14} cm^{-3}$  is the bulk concentration.

With this values

$$\beta = 6.05 V^{-1}.$$

Now it is possible to solve equation 5 and find out that

$$\Psi_s = 0.03 V,$$

this is the silicon surface potential when AZO behaves as a metal. This value complies with equation (1).

#### b) Surface potential when AZO is affected

In this case both AZO and silicon bands bend. Because the dielectric is a perfect insulator and there is not charge in the oxide the charge at both sides of the capacitor have to be the same magnitude both of different sign. Then, because the silicon surface is in depletion and has positive charge the AZO has to be in accumulation and has a negative surface charge.

As already mentioned it has been reported that AZO work function has a big variation, so for this analysis we assume that the Fermi level is under 0.1 eV down the conduction band. This supposition has the only purpose to find out the AZO surface potential. In this case the AZO work function is

$$\varphi_{AZO} = E_{FAZO} + \chi_{SAZO} = 0.1 + 4.5 = 4.6 eV$$

and then,

$$\varphi_{As} = \varphi_{AZO} - \varphi_s = 4.6 - 4.4 = 0.2 eV.$$

Because the Silicon threshold voltage is 0.71 V as previously calculated and  $\varphi_{As}$  is only, 0.2 V the silicon surface is in the depletion regimen.

To start the analysis, as before, we know that the only reason of the band bending is the work functions difference. So equation (1) now is written as:

$$\varphi_{As} = V_{ox} + \Psi_{ss} + \Psi_{sAZO}. \quad (7)$$

Where ss and sAZO are denoting the surface potential in silicon and in AZO respectively.

Now, because there is not charge in the oxide and it is an ideal insulator, the electric field,  $E$ , is constant and it can be written

$$\varepsilon_{ox}E_{ox} = \varepsilon_s E_s = \varepsilon_{AZO}E_{AZO}.$$

Then

$$E_{AZO} = \frac{\varepsilon_s E_s}{\varepsilon_{AZO}}.$$

So,

$$\Psi_{sAZO} = \frac{\varepsilon_s \Psi_{ss}}{\varepsilon_{AZO}} \quad (8)$$

Then equation (7) can be expressed as

$$\varphi_{As} = V_{ox} + \Psi_{ss} + \Psi_{sAZO} = V_{ox} + \Psi_{ss} + \frac{\varepsilon_s \Psi_{ss}}{\varepsilon_{AZO}}$$

or

$$V_{ox} = -\Psi_{ss} \left( 1 + \frac{\varepsilon_s}{\varepsilon_{AZO}} \right) + \varphi_{As}. \quad (9)$$

As before, after some algebra

$$0 = \Psi_{ss}^2 \beta \left( 1 + \frac{\varepsilon_s}{\varepsilon_{AZO}} \right)^2 - \Psi_{ss} \left( 2\beta \left( 1 + \frac{\varepsilon_s}{\varepsilon_{AZO}} \right) \varphi_{As} + 1 \right) + \beta \varphi_{As}^2. \quad (10)$$

Solving this equation and from equation (8), we find

$$\Psi_{ss} = 0.05 \text{ V and } \Psi_{sAZO} = 0.06 \text{ V}.$$

These are the values comply with equation (7), of course it is obviated that they bend in different directions. These are the surface potential of AZO and silicon when both the bands are affected by the work functions difference

and the AZO Fermi level is 0.1 V under the conduction band. Figure 3 shows the AZO and silicon surface potential as a function of the work functions difference due to the AZO Fermi level is assumed to be 0, 01, 02 and 0.3 eV under the conduction band. In all cases, silicon and AZO are in the depletion and accumulation regimen, respectively.

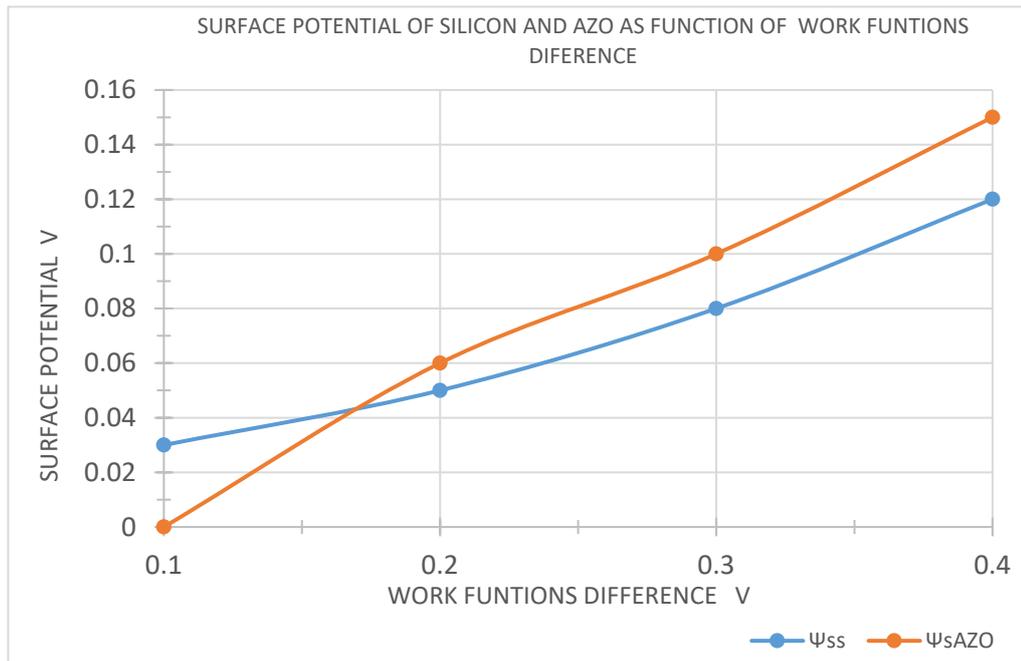


Figura 3. the AZO and silicon surface potential as a function of the work functions difference due to the AZO Fermi level is assumed to be 0, 0.1, 0.2 and 0.3 eV under the conduction band. Take into account that silicon surface is in depletion and AZO surface is in accumulation.

## 2. OXIDE CHARGE EFFECT

Already knowing the effect on the bands due to the work functions difference, we proceed to add the effect due to charge the SRO.

### c) AZO as Metal

As we did in previous section, we start supposing that AZO is so doped that behaves as a metal, and there is not any effect on it. In this case, analyzing

the potentials in the structure the following equation is obtained, again only the magnitude is taking into account. The silicon surface when there are an oxide charge and a work functions difference is:

$$\Psi_{SS}^{ox} = \varphi_{As} + V_{ox} + \frac{Q_t}{C_{ox}} \quad (11)$$

As already calculated when there is not trapped charge, and the AZO behaves as a metal.

$$\Psi_{SS} = \varphi_{As} + V_{ox} = 0.03 \text{ V}. \quad (12)$$

Then

$$\Psi_{SS}^{ox} = \varphi_{As} + V_{ox} + \frac{Q_t}{C_{ox}} = \Psi_{SS} + \frac{Q_t}{C_{ox}} = 0.03 + V_{SRO} \quad (13)$$

Where  $V_{SRO}$  is the voltage in the charged SRO.

It is also known, that the density of traps,  $D_t$ , in Silicon Rich Oxide is, say,  $1 \times 10^{12} \text{ cm}^{-2}$  [10].

Because each trap traps, or releases, one electron the charge (negative or positive) in the SRO is:

$$Q_t = qD_t = 1.6 \times 10^{-19} \text{ coul} \times 1 \times 10^{12} \text{ cm}^{-2} = 1.6 \times 10^{-7} \text{ coul cm}^{-2} \quad (14)$$

Because we want the silicon surface to be in depletion regimen, negative charge has to be supplied to the SRO. Then

$$V_{SRO} = \frac{Q_t}{C_{ox}} = \frac{1.6 \times 10^{-7}}{1.1 \times 10^{-8}} = 14.5 \text{ V} \quad (15)$$

again the sign was ignored. So

$$\Psi_{SS}^{ox} = 0.03 + V_{SRO} = 0.03 + 14.5 = 14.53 \text{ V} \quad (16)$$

So, the silicon surface is in inversion when all SRO traps are filled with electrons and the AZO behaves as a metal.

d) AZO = 0.1 eV under the conduction band

Let's see the case when AZO is 0.1 eV under the conduction band. In this case, the silicon surface potential is determined by the charge in the SRO and  $\varphi_{As}$ ,

$$\psi_{ss}^{ox} = \varphi_{As} + V_{ox} + \frac{Q_t}{C_{ox}} = \psi_{ss} + \frac{Q_t}{C_{ox}} \quad (17)$$

As already calculated,

$$\psi_{ss} = 0.05 \text{ V} \quad (18)$$

Then, the surface silicon potential when the AZO fermi level is under 0.1 eV under the conduction band is:

$$\psi_{ss}^{ox} = \psi_{ss} + \frac{Q_t}{C_{ox}} = 0.05 + 14.4 = 14.45 \text{ V}. \quad (19)$$

So when AZO has the fermi level 0.1 eV under the conduction band there is a work functions difference, the doping in silicon is  $1 \times 10^{14} \text{ cm}^{-3}$ , and the SRO is completely charged, then the silicon surface in inversion regimen. That is because we are charging the SRO negative, as a consequence the silicon surface has a positive charge and the surface potential is higher than the  $V_t$ .

e) Azo surface potential

Again the AZO surface potential is dominated by the charge in the SRO and the work functions difference, Then

$$\psi_{sAZo}^{ox} = \psi_{sAZO} + \frac{Q_t}{C_{ox}}. \quad (20)$$

$\psi_{sAZO}^{ox}$  is the surface potential when there is a difference between work functions and also there is an oxide charge, and  $\psi_{sAZO}$  is the surface potential due to the difference of work functions. The last term is the effect of the charge in the oxide. As already calculated

$$\psi_{sAZO} = 0.065, \text{ and } V_{SRO} = 14.5 \text{ V}$$

Then

$$\Psi_{sAZO}^{ox} = \Psi_{AZO} + \frac{Q_t}{C_{ox}} = -0.065 + 14.5 = 14.44 \text{ V} \quad (21)$$

The minus sign is because the band bending due to the difference in work functions is contrary to that produced by the SRO negative charge.

Then, surface potential of AZO when all SRO traps are negatively charged, and the AZO Fermi level is 0.1 eV under the conduction band is

$$\Psi_{sAZO}^{ox} = 14.44 \text{ V.}$$

#### iv. Minimum charge to form a depletion zone

##### f) In the silicon surface

The surface inversion layer starts when the surface potential is equal to the potential in the bulk,  $\Psi_B$ . So, in this stage it is assured that there is a depletion layer formed. As already calculated, for  $N_B = 10^{14} \text{ cm}^{-3}$ ,

$$\Psi_B = 0.23 \text{ V.}$$

Then, when the AZO behaves as a metal

$$\Psi_{ss}^{ox} = \Psi_B = 0.23 \text{ V} = \Psi_{ss} + \frac{Q_t}{C_{ox}} = 0.03 + \frac{Q_t}{C_{ox}} = 0.03 + V_{SRO} \quad (22)$$

Clearing  $V_{SRO}$ ,

$$V_{SRO} = \frac{Q_{SRO}}{C_{ox}} = 0.23 - 0.03 = 0.2 \text{ V} \quad (23)$$

now

$$Q_t = 0.2 \times C_{ox} = 0.2 \text{ V} \times 1.1 \times 10^{-8} \frac{\text{F}}{\text{cm}^2} = 2.2 \times 10^{-8} \frac{\text{coul}}{\text{cm}^2} \quad (24)$$

So any charge that is higher than  $2.2 \times 10^{-8} \text{ coul cm}^{-2}$  will produce a silicon surface depletion, this means that charging with negative charge higher than 14 % of the SRO traps a depletion layer is granted in the silicon surface.

g) In the AZO surface

In the same way for AZO it is known that the band gap for AZO is 3.3 eV and then the AZO intrinsic fermi level is at 1.65 eV. If we assume that the AZO fermi level is 0.1 eV under the conduction band. Then the Surface potential should be 1.55 eV. So, using equation (22) and (24) for AZO:

$$\Psi_{AZO}^{ox} = 1.55 = \Psi_{sAZO} + \frac{Q_t}{C_{ox}} = -0.065 + \frac{Q_t}{C_{ox}}, \quad (25)$$

and

$$Q_t = (1.55 + 0.065) \times C_{ox} = 1.61 \times 1.1 \times 10^{-8} = 1.8 \times 10^{-8} \frac{\text{coul}}{\text{cm}^2} \quad (26)$$

So any charge that is higher than  $1.8 \times 10^{-8} \text{ coul cm}^{-2}$  will produce an AZO surface depletion, Considering, that the total charge in the SRO is  $1.6 \times 10^{-7} \text{ coul cm}^{-2}$ , this means that charging the SRO with negative charge higher than 11 % of the SRO traps a depletion layer is formed in the AZO surface.

To have both silicon and AZO surfaces in depletion regimen it is necessary to charge the SRO with at least  $2.2 \times 10^{-8} \text{ coul cm}^{-2}$ .

### 3. Conclusions

An analysis of a Semiconductor/Insulator/Semiconductor capacitor was done in order to obtain the condition needed to have both semiconductors simultaneously in depletion mode. It was found that using AZO/SRO/Si structure it is possible to have both AZO and Si simultaneously in depletion just charging the SRO negatively. This opens the door to have two solar cells in the same structure and use them in tandem. This of course will improve the efficiency of the system.

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