Impact of Interface Traps and Zn Diffusion on Performance of Lateral Hybrid III-V/Si Photodetectors

Q. Ding[1], Y. Baumgartner[2,3], L. Czornomaz[2], A. Schenk[1]
[1]Integrated Systems Laboratory, ETH Zurich, Zurich, 8092, Switzerland
[2]IBM Zurich Research Laboratory, Rüschlikon, 8803, Switzerland
[3]Institute of Quantum Electronics, ETH Zurich, 8093, Switzerland
e-mail: dingq@iis.ee.ethz.ch

Abstract

This paper attempts to gain insight into the physical mechanisms related to device performance of a recently reported hybrid III-V/Si waveguide-coupled photodetector with lateral current collection (LCC-PD) using coupled 3D optical and 2D electrical simulations. We demonstrate that Zn diffusion, a widely observed phenomenon for p-doped III-V materials, could increase the dark current and lower the responsivity. We also show that the dark current at low bias is related to e-type interface traps near the bottom of the n-i junction.
(Keywords: LCC-PD, Zn diffusion, interface traps**)**

Introduction

CMOS-compatible photodetectors with high speed and low power consumption are key components for on-chip optical interconnects. Recently, a new-generation waveguide-coupled hybrid III-V/Si LCC-PD has been designed and fabricated at IBM-Research Zurich [1]. The device utilizes the LCC scheme to decouple optical and electrical designs by separating light propagation direction from carrier collection direction, as shown in Fig. 1 (a). The light-absorbing medium consists of intrinsic InAlGaAs multiple quantum wells (MQWs) with ten well/barrier pairs. The MQW stack is trapezoidal-shaped, with the bottom being 300 nm wider than the top due to dry etching, whereas the coupled InP WG has the same width as the MQW top. An InAlGaAs separate confinement heterostructure (SCH) layer and an InP clad layer are used for better optical confinement. Contact regions are composed of highly doped InP with a concentration of 1.3e19 cm^{-3} (3e18 cm^{-3}) for the n-type (p-type) region. All intrinsic III-V material regions are assumed to be slightly n-doped with a concentration of 2e16 cm^{-3}. Other details about the structure are sketched in Fig. 1 (b), where the triangular i-InP regrown regions

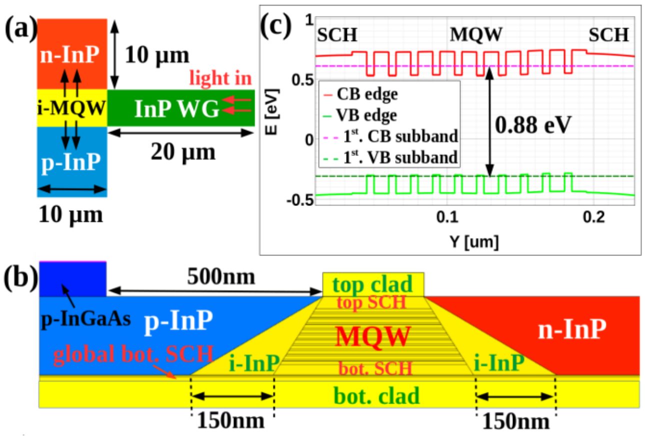

Figure 1: (a) top view of studied device, where red (black) arrows indicate the light propagation (carrier collection) direction. (b) sketch of cross section along the carrier collection direction. (c) band diagram along MQW stack with the energy gap between the 1st CB and 1st VB subband being 0.88 eV.

and the global bottom SCH layer are present as consequence of fabrication requirements. Further information about the material composition and layer thickness in the MQW stack is listed in Table 1. Band structure calculations using *Sentaurus S-Band* based on the 6-band k·p method were performed to confirm the MQW effective band gap (~0.88 eV) obtained in experiments (Fig. 1 (c)). Relevant material parameters used in these calculations are taken from Ref. [2].

TABLE 1. Material composition and layer thicknesses

Region	Material composition	thickness [nm]
quantum well	$In_{0.62}Al_{0.14}Ga_{0.24}As$	5
quantum barrier	$In_{0.49}Al_{0.29}Ga_{0.22}As$	10
top SCH layer	$In_{0.53}Al_{0.3}Ga_{0.17}As$	35
top clad layer	InP	15
bot. SCH layer	$In_{0.53}Al_{0.3}Ga_{0.17}As$	30
bot. clad layer	InP	15
global SCH layer	$In_{0.53}Al_{0.3}Ga_{0.17}As$	5

Record-level performance of these devices has been demonstrated, such as low dark current in the nA range, high bandwidth exceeding 35GHz and ultralow capacitance of few fF. However, the photo responsivity turned out to be relatively low (below 0.5 up to a bias of -10 V) even after optimization of the optical design [1]. In order to find out the reason and further improve the performance, the flow of the dark and photo currents must be explored. To do this, we first perform 2D electrical simulations using *Sentaurus Device* to reproduce the measured dark current. The discovered physical mechanisms from the dark current study are used as initial setup in the subsequent study of the photo responsivity, where 3D FDTD simulations using *Sentaurus EMW Solver* are coupled with 2D electrical simulations to calculate the photo current and qualitatively analyze possible origins of the low responsivity. The coupling is achieved by extracting a 2D photo generation profile obtained from 3D optical simulations as input for the 2D electrical simulations. This profile is obtained by cutting the 3D structure in plane normal to light propagation direction at middle MQW. Such an approach is reasonable in our case because the extension of the MQW region in light propagation direction (10 µm) is much longer than the targeted wavelength (~1.41µm), but still too short to cause a significant optical intensity decay in absorbing regions. In the 2D electrical simulations, the Shockley-Read-Hall (SRH) lifetime is set to 1 ns for all III-V materials, and a field dependence of the SRH lifetime (trap-assisted tunneling) is included using the default Schenk's model in *Sentaurus Device*.

Dark Current Analysis

The dark current in photodetectors should be kept as low as possible to reduce the shot noise in photodetection. Understanding the physical origin of the dark current is essential to improve the electrical design. Several effects contributing to the dark current flow have been reported, such as trap-assisted tunneling and band-to-band tunneling [3] [4]. Here, we show that the dark current in the studied device is mainly related to Zn diffusion and electrostatic effects originating from InAlGaAs/InP interface traps at specific locations.

A. *Impact of Zn Diffusion*

Zn diffusion is a commonly observed phenomenon in p-type III-V semiconductors [5]. In the studied device, we

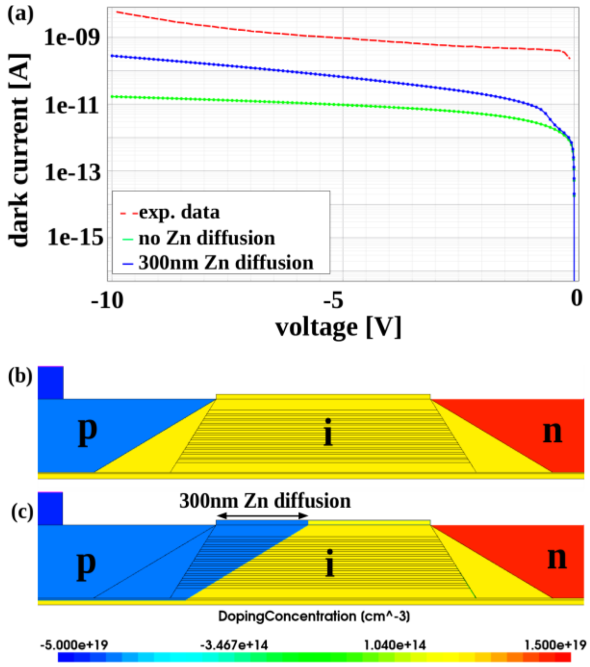

Figure 2: (a) dark IV curves from experiment (red dashed curve) and simulations, without (green solid curve) and with 300 nm Zn diffusion (blue solid curve). Doping profile in device (b) without and with (c) 300 nm Zn diffusion.

estimate a Zn diffusion of 300 nm towards the absorbing medium with a uniform p-doping concentration of 3e18 cm^{-3} based on experimental Secondary Ion Mass Spectroscopy (SIMS) analysis. To study its impact on device performance, we simulated a device with a top MQW width of 700 nm and found that Zn diffusion could increase the dark current, as shown in Fig. 2 (a). The reason for this higher dark current is that Zn diffusion along the carrier transport direction turns the entire left regrown i-InP region and some left parts of the intrinsic MQW stack into p-doped (Fig. 2 (b) (c)), which shifts the pi-junction towards the n-contact region, and thus enhances the electric field in the remaining intrinsic region not affected by Zn diffusion (Fig. 3). This effect is stronger as MQW's dimension along transport direction becomes smaller. Therefore, the unintentional Zn diffusion in III-V compounds could be an obstacle to further miniaturization of p-i-n type photodetectors.

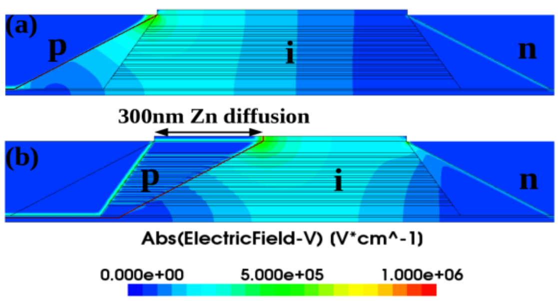

Figure 3. Electric field profile at -10V (a) without and (b) with 300 nm Zn diffusion. Color bar ranges from 0 to 1e6 V/cm.

B. Location of Interface Traps

Though Zn diffusion leads to a higher dark current, the simulated values are still lower than the experimental data, especially at small reverse bias, as seen in Fig. 2 (a). Hence, another contributing mechanism must exist. It is found to be related to changes in the electrostatics due to interface traps at specific locations. To study this dependency, we included traps at different interface sections separately and compared the simulated dark current with the experimental data. The trap parameters used are based on measurements reported in Ref. [6]. Electron-type traps at the InP/InAlGaAs interface with a concentration of 3e13 $eV^{-1}cm^{-2}$, a center trap energy level at 0.43 eV below the conduction band edge, and a 0.3 eV wide Gaussian shaped broadening window are assumed.

With these assumptions, the impact of interface traps in three regions is studied in this work, including the left and right regrown InP regions and the global bottom SCH layer. This approach considers the high probability of traps existing in a real device due to its complex structure. The comparison of the simulated dark IV curves with experimental data (Fig. 4) indicates that traps located at the interface between global bottom SCH layer and right InP regrown region are the most relevant for the observed high dark current at small bias.

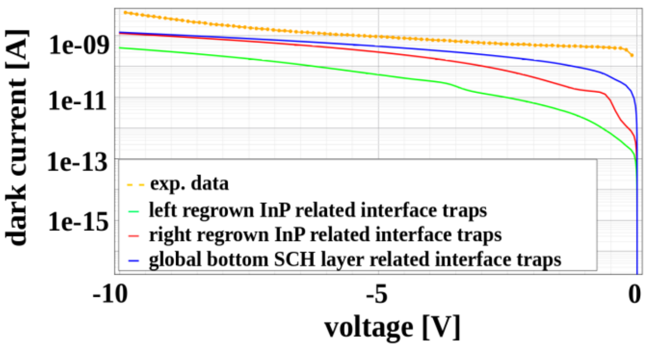

Figure 4: dark IV curves from experiment (orange dashed curve) and simulations assuming traps located at InAlGaAs/InP interfaces related to left (green solid curve) and right (red solid curve) regrown InP region and the global bottom SCH layer (blue solid curve).

This finding can be explained as follows. The assumed high-concentration electron traps, which act as deep acceptors, lead to a transition of the bottom right regrown InP and global bottom SCH layers from slightly n-doped (intrinsic) to p-type, causing the formation of a built-in pn-junction between these regions and the highly doped n-InP contact region, as shown in Fig. 5 (a). This built-in junction results in a higher built-in electric field, thus a higher current flow at low bias (Fig. 5).

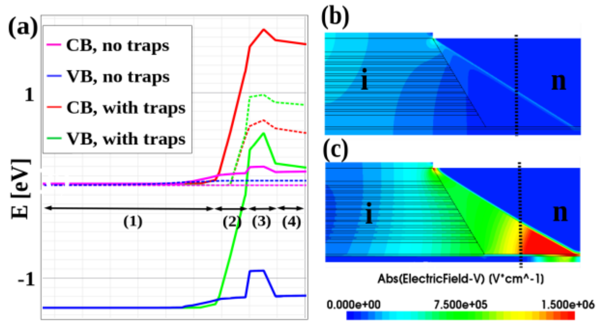

Figure 5: (a) band diagrams without traps and with interface traps related to global bot. SCH layer, cutting vertically along (1) n-InP, (2) right regrown InP, (3) global bot. SCH and (4) bot. InP clad region. Dashed lines are electron (hole) Fermi levels, with same color used for corresponding CB (VB) edge. Electric field profile at -1V in case of (b) no traps and (c) global bot. SCH related interfaces traps. Black dashed line shows vertical cut used in (a). Color bar ranges from 0 to 1.5e6 V/cm.

Responsivity Analysis

Besides the dark current, the photo responsivity is an important feature of photodetectors. Defined as the ratio of photocurrent and input optical power, it indicates the collection efficiency of photo-generated carriers. Any poor optical, electrical, or coupling design could cause a low responsivity. In this work, we propose possible origins of the observed low responsivity by simulating and analyzing the photo current flow. The studied device has a MQW top width of 300 nm. Two reasons for the low responsivity are found: (i) the opto-electrical profile mismatch in the light absorbing region caused by Zn diffusion and (ii) the large valence band offset at the InAlGaAs/InP interface, which leads to inefficient hole collection. Details are discussed in the following.

A. Opto-electrical Profile Mismatch

A high responsivity in photodetectors requires that most of the photo-generated electron-hole pairs are efficiently separated and collected at the corresponding electrode. This separation process mainly relies on the drift field in the carrier-generation region. Therefore, a low or even absent electric field in this region can lead to a low responsivity even under high optical generation. The geometrical profile mismatch between optical generation rate and electric field is known as the *opto-electrical profile mismatch*. It is found to be one origin for the relative low responsivity observed in the studied device, and its occurrence is due to the aforementioned impact of Zn diffusion. As discussed before, Zn diffusion turns the left part of the originally intrinsic MQW into p-doped and shifts the pi-junction to the right. Consequently, the former electric field in this region disappears and the carriers generated here are not able to be extracted even under a high reverse bias up to -10V, as observed in experiments (Fig. 6).

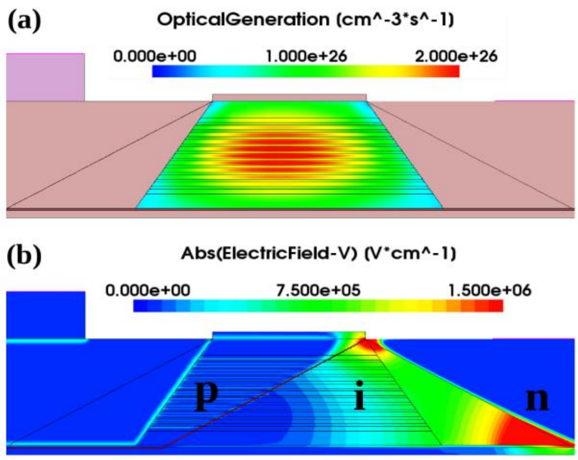

Figure 6: (a) optical generation rate and (b) electric field profile at -10V in device with 300 nm MQW top width, assuming 300nm-long Zn diffusion.

B. High Valence Band Offset Barrier

The opto-electrical profile mismatch emphasizes the requirement of a high drift field for efficient separation of generated carriers. In order to contribute to current flow, the separated carriers need to travel to the contact region and reach the electrodes. Thus, any effect that impedes carrier transport from the generation region to the electrode can also lower the responsivity. The main obstacle related to this collection process is found to be the high valence band offset barrier at the InP/InAlGaAs interface (~0.3 eV), as shown in Fig. 7 (a). Thus, holes generated in the MQW region are unable to overcome this barrier and reach the anode through the left regrown InP region. Instead, they are forced to flow along this high-barrier interface down to the thin global bottom SCH layer (Fig. 7 (b)). This narrow flow path causes current crowding and lowers the carrier collection efficiency, and thus the responsivity. Furthermore, the resultant high resistance might limit its operation speed.

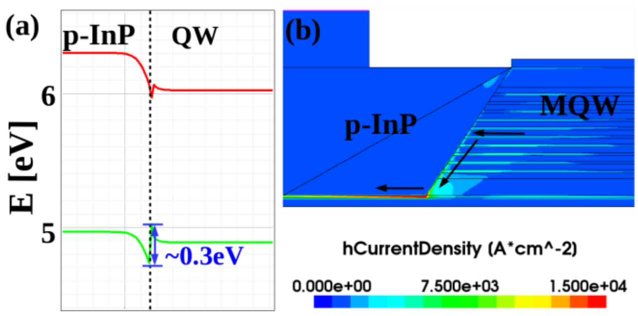

Figure 7: (a) band diagram at InAlGaAs/InP interface, obtained by a cut along the transport direction through p-InP and 1st. quantum well. (b) hole current density profile at -5V near this region.

Conclusion

We demonstrated that Zn diffusion and InP/InAlGaAs interface traps at specific locations can degrade the performance of p-i-n type photodetectors by simulating recently reported waveguide-coupled MQW LCC-PDs. We showed that Zn diffusion causes a higher dark current due to a resultant higher electric field in the narrowed intrinsic region. This phenomenon is also found to be one reason for the observed low responsivity, as it causes geometrically mismatched profiles between optical generation rate and electric field. Another reason is the high valence band offset barrier at the InP/InAlGaAs interface. We also found that the high dark current at small bias is most likely caused by electron-type interface traps located at the interface between global bottom SCH layer and right regrown InP region due to the formation of a built-in pn-junction. Thus, we suggest that methods to control Zn diffusion and to improve the material interface quality could be taken in order to achieve further performance enhancement.

Acknowledgement

The authors thank Dr. Saurabh Sant, Infineon Technologies AG Munich, for useful discussions.

References

[1] Y. Baumgartner et al, "Novel CMOS-Compatible Ultralow Capacitance Hybrid III-V/Si Photodetectors Tested up to 32 Gbps NRZ," Optical Fiber Conference (OFC) (2019).

[2] I. Vurgaftman et al, “Band Parameters for III-V Compound Semiconductors and Their Alloys”, Journal of Applied Physics 89, 5815 (2001).

[3] X.L. Ji et al, “2.6µm MBE Grown InGaAs Detectors with Dark Current of SRH and TAT”, AIP Advances 4, 087135 (2014).

[4] M. Verdun, “Dark Current Investigation in Thin P-i-N InGaAs Photodiodes for Nano-resonators”, Journal of Applied Physics 120, 084501 (2016).

[5] Y. Huang, “Control of Zn Diffusion in InP/InAlGaAs-based Heterojunction Bipolar Transistors and Light Emitting Transistors”, Journal of Crystal Growth 310, 4345–4350 (2008)

[6] Z.C. Huang, “Interface Traps in InP/InAlGaAs p-n Junctions by metal organic chemical vapor deposition”, Journal of Applied Physics 77, 5736 (1995).