Characterization of Zinc oxide Contact on Metal Substrates using Low-Cost Fabrication Techniques and TCAD

Priyadarshini Jena*, Rajesh Ku Mishraa, K.Hari Krishnaa

*Department of ECE Engineering, CUTM, Paralakhemundi, Odisha
bDepartment of EIE Engineering, CUTM, Paralakhemundi, Odisha


Abstract

In this project we present the modelling and simulation of ZnO contact on metal substrates using SILVACO TCAD Tool. SILVACO Software is a 2D simulation tool used for modelling and fast simulation of all types of semiconductor devices. It provides two simulators-Athena and Atlas. ZnO is a compound semiconductor with a wide band-gap used for various fields of optoelectronics, sensors and nanotechnology. The model for ZnO contact on metal substrates like (Al, Cu) interaction showed the effect of ZnO, its stability of contact formation and electrical characteristics. ZnO being a compound semiconductor it’s challenging to produce rectifying characteristics over metal substrates. This was possibly obtained through Silvaco. Both the electrical and material characterization of ZnO on metals were analysed and studied. This project proposed an easy and low-cost characterization that was able to emphasize the model designing in Silvaco Software. The stable contact formation of ZnO attracted further in various high-frequency applications. All simulated results and the experimental results evolved are comparatively analysed and studied. Experimental results are taken inputs for the simulators –Atlas which ultimately proved and showed the models functioning properly. Advantages of Modelling—Easy and fast simulation in order to cope up with real-time fabrication methods.

Keywords: Silvaco-atlas, ZnO, Rectifying Characteristics, Sensor, Nanotechnology.

1. Introduction

Now days the Semiconductor technology has increased a lot and it has shown that the knowledge of different materials plays a key role in the fabrication of these devices. The science dealing with the study of properties of materials is Material Science. This it has made it possible the fabrication, modelling and simulation of these semiconductor devices. The available and implement of low-cost and easy fabrication methods will attract many researchers to design out the structures and model in technological oriented simulation tools like SILVACO. Based on these background the objective of this work was study and analysis of certain materials including their behavioural properties like conductivity, resistivity and mobility etc. Then performing experiments on these materials to fabricate and simulation using TCAD tool called SILVACO. So ultimately a device model of an aluminium substrate with Zinc oxide deposition was studied. This modeling was possibly done through TCAD Simulation tool. So main focus was study of materials i.e selection of Aluminium metal as the substrate and Zinc oxide deposition. These user-friendly tools nowadays made the fabrication processes easy to perform without any complexity.

The characterisation obtained through these tools enhances the performance and running of devices more accurately. Very frankly, even if no fabrication machinery and instruments are unavailable these tools helps out a lot in carrying out the fabrication processes. As we know all semiconductor technology has led to development of all Si-related devices. Here ZnO is a new and exotic semiconductor with a wide band-gap, due to its wide band-gap its really tough to extract electrons from its valence band to conduction band. ZnO has in fact been in use for thousands of years. ZnO initially was focused on contact formation over metal substrates like Aluminium and Copper. These metals are easily available and of very low-cost. We are very well aware the electrode potentials of these metals. Most of the study was on depositing ZnO over metals with proper dimensions using easy and low-cost methods like sol-gel preparation. The whole system model is designed using SILVACO software. It provides fast simulation and accurate results for all critical fabrication steps. It has ability to produce 2D structure and a cross-section 1D structure too. In the other hand Atlas simulator is used to design all solid-state devices. Results

* Corresponding author’s Email: priyadarshini@cutm.ac.in
from physical design will be used as inputs by Atlas whereby it will estimate the physical properties of the device as per the model made in Silvaco.

Fig. 1 Cross-sectional figure

The above fig1 shows the cross sectional figure used in modelling the contacts between ZnO and metal substrates (Al, Cu). Hardware development involves design and development of ZnO, along with collection of materials in order to perform the experimental procedures.

2. Experimental materials and methods

First of all experimental methods are carried out for contact formation between ZnO and the subsequent metals i.e Aluminium, and Copper then their results are taken as inputs for Atlas-simulator (SILVACO) to get the simulated output results. For this we require proper deposition of ZnO over metals. The methods used for characterisation of ZnO- four – probe method, Hall Effect method etc. The chemically wet and dry method provides the low-cost method for the growth of zinc oxide over metal substrates like aluminium, copper etc. The proper deposition of the solution over the metals must be carried out carefully. After deposition it is then cooled through other low-cost fabrication equipments where characterization of those metal substrates was done to find the results. The initial step was preparation of ZnO using sol-gel method. The sol-gel method was carried out low-cost fabrication technique called Chemically Wet and Dry method (CWD) whose set-up was shown in figure below. CWD is a film growth process in Chemically Wet and Dry technique which is the mass transport of the reactant performed in the vapour phase. The oxide semiconductor thin films play an important role in electronic device technology. Of late, the oxide coatings of mechanical cutting tools are commercially very useful for longer tool-life. The CWD (Chemically Wet and Dry) equipment presently developed can produce oxide films in an inexpensive way for the following specific applications in electronic and other related fields.

All the metals – Aluminium, Silver and Copper was cut into strips all in equal dimensions. After this ZnO solution was deposited over these metals through spin-coating and dried and annealed through hot-air oven. These devices are allowed for carrying out low-cost fabrication processes. All these samples are characterised through four-probe method, Hall Effect thereby extracting parameters like resistivity, mobility and conductivity etc along with graphs.

3. Experimental results

The figure shows the whole material characteristics of the contacts between ZnO and the metal substrates. The overall characterization was done using four-probe and Hall Effect method. The characteristics of current and voltage was almost found and rectifying with initially constant then almost increases rapidly. The four probe method helps in determining the Current-Voltage characteristics. The Hall Effect helps us in determining the type of semiconductor i.e. whether n-type or p-type and the resistivity and other calculations like conductivity, mobility calculation values can be obtained. The Graphs Fig 2 and Fig 3 below shows the characteristics for Al-ZnO and Cu-ZnO, obtained from four probe method to calculate the resistance, hall-coefficient etc. These methods provide an easy way for determining the results. These results were taken as inputs for the simulation software for exact simulated output characteristics.

4. Materials and methods in Silvaco

In this study, the structure development of current contact between Semiconductors (ZnO) with metal substrates in 2D in Silvaco is essential. On top of the metal substrate, ZnO was deposited as the coating layer. The model was done following the schematic figure as in Fig. 1. The first step of this project is to model the structure as shown in fig1 with proper dimensions then voltage will be applied to the anode part for determination of I-V characteristics. For this we need to write the code for I-V characteristics and then simulate the code. Resistance can be calculated from the above. This code was written by applying voltage
to the anode electrode i.e ZnO semiconductor to check its exact functioning as ZnO is a wide-gap semiconductor it’s difficult to extract electron from valence band to conduction band. Aluminum has got a work function of around 4.3ev this has to be mentioned in the code for simulation of the code. Here after simulation we obtained the rectifying characteristics as shown in the figure below. Similarly Copper has got work function of 5.4ev which is higher than Aluminum. The same code was followed in case of copper. The rectifying characteristics for Cu-ZnO contact was obtained as shown in the figure below:

5. Simulated results and discussions

The rectifying characteristics for both the metals are obtained through SILVACO TCAD where we can have a comparison between their simulated values and their experimental values of the metal substrates. We can see how zinc oxide shows reactive over aluminium as well as copper metal.

In this project it was expected that the current-voltage characteristics obtained in Silvaco in case of Copper is quite higher than Aluminum case. The calculations i.e. resistivity, conductivity values obtained during hall-effect and four-probe methods are quite more than Aluminum. This was analyzed (I-V) curve and extraction of other physical parameters is specified in the coding itself. A comparative study between the experimental and simulated results can be done. A similar trend of characteristics was analyzed from the device modeled in Silvaco and experimental procedures.

Conclusions

This project is initiated to make use of these TCAD tools for designing and modelling devices using fabrication methods. It fulfils the objective to those that are followed by using real time fabrication methods which of high cost and complex in carrying out the processes. The study and learning of tools successfully makes the system easy in determining and visualising the results. The knowledge of different materials plays a key role in the fabrication of these devices. The science dealing with the study of properties of materials is Material Science. This itself has made it possible the fabrication, modeling and simulation of these semiconductor devices. The availability and implementation of low-cost and easy fabrication methods will attract many researchers to design out the structures
and model in technological oriented simulation tools like SILVACO. The low-cost technological processes has motivated the researchers to go for implementation of semiconductor devices using such design tools. These methods can fulfill the objective of carrying out the processes with new and advanced semiconductor devices. The dip-coating method helps out in development and running of devices in simulated form. As the mechanism are cost-effective and easily available.

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