USING THE TAGUCHI METHOD TO PROPOSE A MATHEMATICAL MODEL FOR STUDY THE DEPOSITION OF DOPED ZnO NANOPARTICULES

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Abstract: The nanoscaled semiconductor are used in recent years in manufacturing electronic and optoelectronic devices. One of the most important transparent conducting oxides is ZnO in nanoscale configuration. This oxide has been used as highly transparent conducting layers in place of some expensive films in flat panel displays and photovoltaic devices.
In our work we proposed a mathematical model, based on the Taguchi method, for study the deposition of doped ZnO nanoparticules.

INTRODUCTION

Recent improvements in the control of background conductivity of ZnO and demonstrations of n-type doping have intensified interest in this material for applications in UV light emitters, varistors, transparent high-power electronics, surface acoustic wave devices, piezoelectric transducers, and chemical and gas sensing. ZnO has several potential advantages over GaN for some of these applications, including the commercial availability of bulk single crystals and a larger exciton binding energy (~60 meV compared with ~25 meV for GaN). The latter property should translate to even brighter light emission than obtained with GaN photonics.
To realize any type of device technology, it is important to have control over the concentration of intentionally introduced impurities, called dopants, which are responsible for the electrical properties of ZnO. The dopants determine whether the current (and, ultimately, the information processed by the device) is carried by electrons or holes. In semiconducting oxides, it is generally possible to achieve one or other of these types, but not both.
The dopants are also called shallow level impurities because they introduce energy levels close to one of the allowed energy bands in the material and are easily ionized as a result. There may also be unintentional impurities introduced during the growth of ZnO that have a deleterious effect on the properties of the material.

TECHNIQUES OF DEPOSITION

Using techniques such as pulsed laser deposition (PLD), molecular beam epitaxy (MBE), or even reactive sputtering, ZnO of reasonable quality can be deposited at lower growth temperatures than GaN.
This leads to the possibility of transparent junctions on cheap substrates such as glass, with the potential to realize low-cost UV lasers or light-emitting diodes for high-density data storage systems, solid-state lighting (where white light is obtained from phosphors excited by blue or UV light-emitting diodes), secure communications, and biodetection. ZnO is a direct band gap semiconductor with Eg = 3.4 eV. The band gap of ZnO can be tuned via divalent substitution on the cation site to produce heterostructures. Cd doping can decrease the band gap (to as low as ~3.0 eV), whereas Mg doping can increase the band gap (to as high as ~4.0 eV).
ZnO normally forms in the hexagonal (wurtzite) crystal structure with a = 3.25 Å and c = 5.12 Å. Electron doping in nominally undoped ZnO has been attributed to Zn interstitials, oxygen vacancies, or hydrogen. The intrinsic defect levels that lead to n-type doping lie approximately 0.01-0.05 eV below the conduction band.

The optical properties of ZnO, studied using photoluminescence, photoconductivity, and absorption reflect the intrinsic direct band gap, a strongly bound exciton state, and gap states arising from point defects.
A strong room temperature, near-band-edge UV photoluminescence peak at ~3.2 eV is attributed to an exciton state, as the exciton binding energy is on the order of 60 meV. In addition, visible emission is also observed as a result of defect states. For ZnO, n-type conductivity is relatively easy to realize via excess Zn or with Al, Ga, or In doping, but p-type doping has only recently been achieved. This is a fairly common occurrence in wide band gap semiconductors8, where difficulty in achieving bipolar (n- and p-type) doping is not unusual. ZnSe and GaN can be easily doped n-type, while p-type doping is difficult. In contrast, ZnTe is difficult to dope n-type, while p-type doping is easily achieved.

EXPERIMENTAL AND CARACTHERISATION

The ZnO powders doped with different quantities of Al were obtained using Zn(NO3)2 and AlCl3 as precursors and KOH as hydrolysis agent.

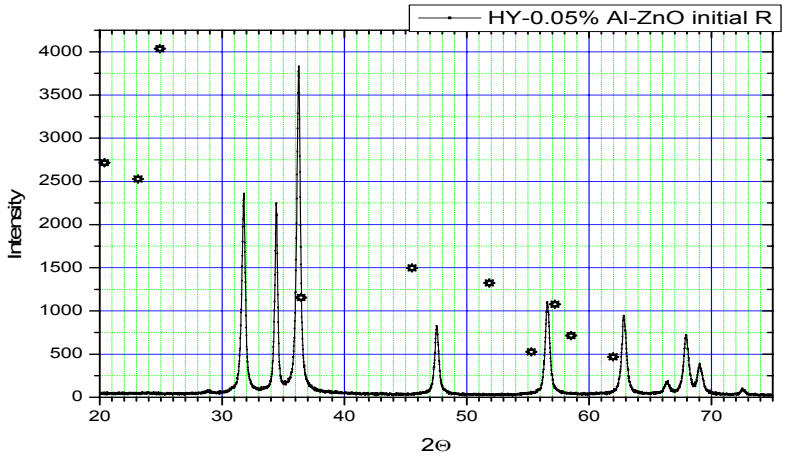

Fig 1. XRD of 0,05%Al doped ZnO nanoparticules

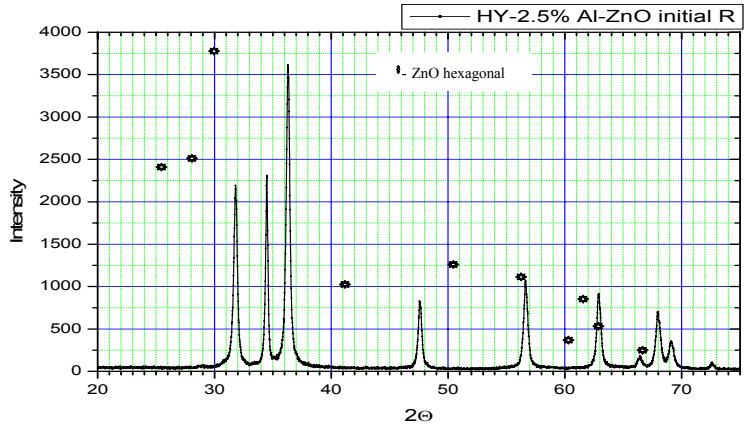

Fig 2. XRD of 2,5%Al doped ZnO nanoparticules

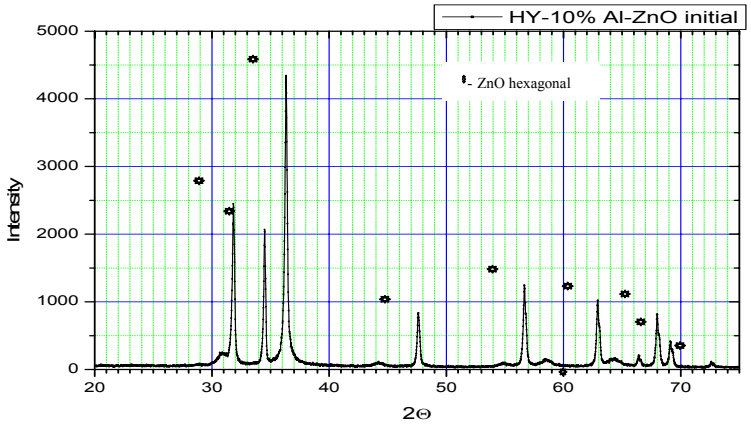

Fig 3. XRD of 10%Al doped ZnO nanoparticules

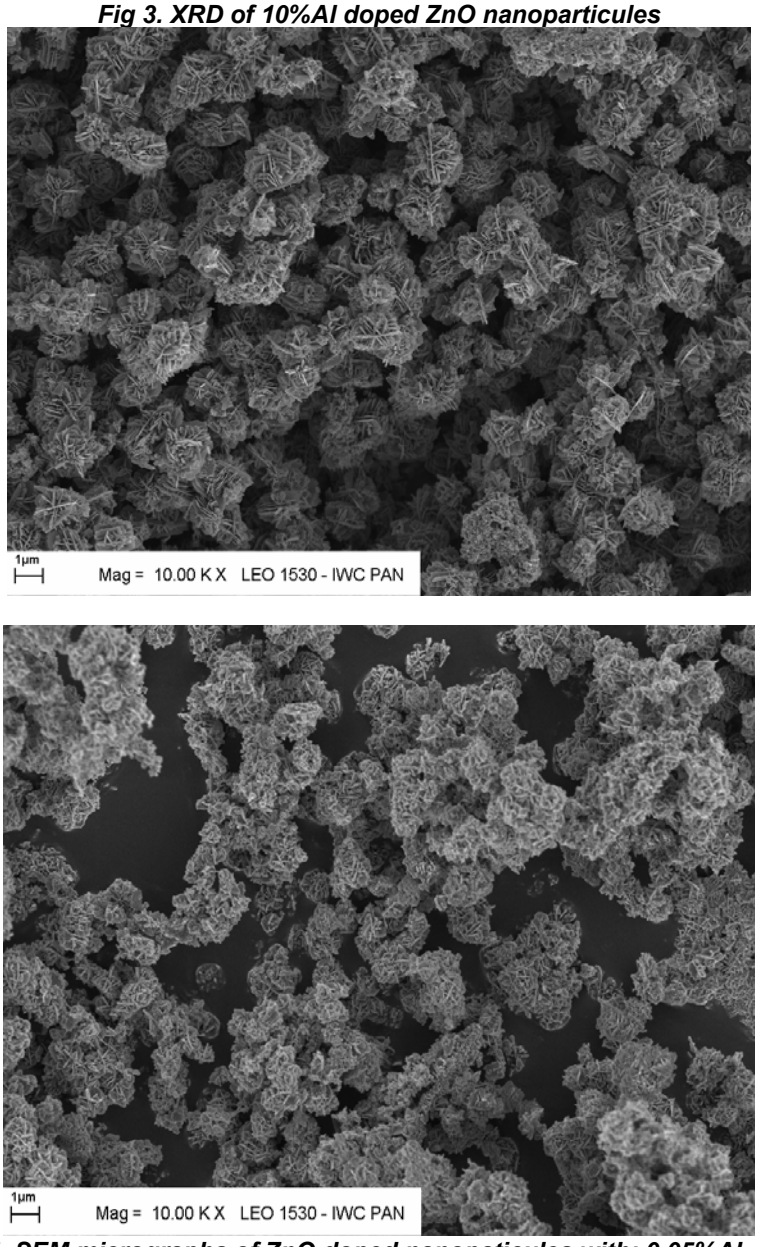

Fig 4. SEM micrographs of ZnO doped nanopaticules with: 0,05%Al, 1%Al

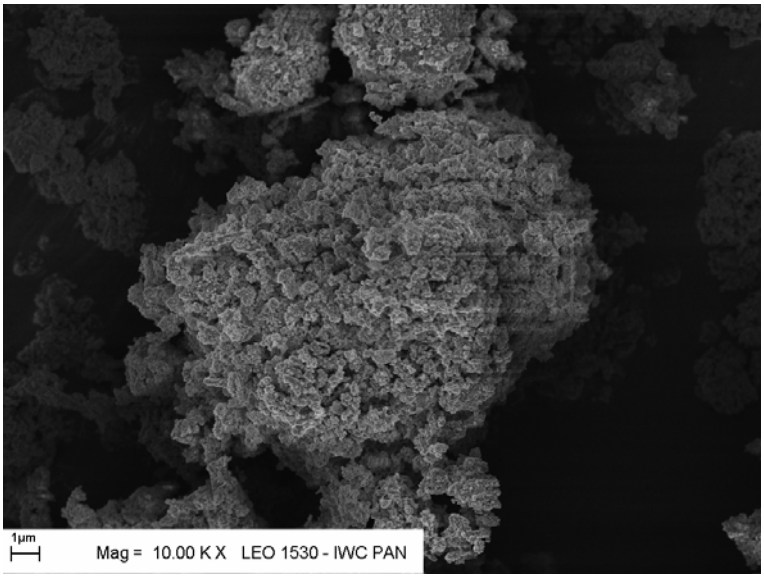

Fig 5. SEM micrographs of ZnO doped nanopaticules with 10%Al

A MODEL TO STUDY THE DEPOSITION OF DOPED ZnO NANOPARTICULES PROCESS

These nanoparticles are used relatively in the nanoelectronics industry.
By the Taguchi method, we are identified the factors of process:
These factors are:

- the size of ZnO molecules compared with those of GaN;
- the conductivity properties;
- the transparency;
- the cost;
- the excitation energy;

In order to modeling the process function of ZnO nanostructured powders, we define the function as:
$I = f(x_1, x_2, \ldots, x_n)$;
Where:
I- the deposition function;
$x_1, x_2, \ldots, x_n$ - the factors of influence;
The schema of deposition process in shown in figure 6.

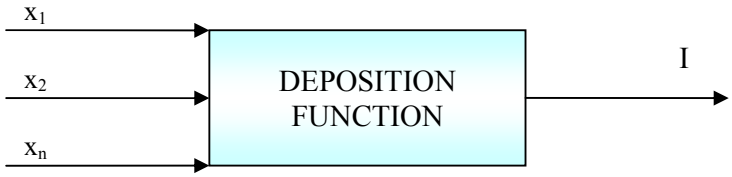

Fig 6. The schema of the impact function

The mathematical model is:
$I = k \cdot x_1^{\ a} \cdot x_2^{\ b} \cdot \ldots \cdot x_n^{\ t}$,
We have:
Variable: $x_1, x_2, \ldots, x_n$ – known;
Constants: k, a, b,…,t – unknown;

By a logarithmic transformation we obtain a linear form:
$\lg I = \lg k + a \lg x_1 + b \lg x_2 + \ldots + t \lg x_n$
We transform:

$\lg I = Y$	$\lg k = A0$
$\lg x_1 = X1$	$a = A1$
$\lg x_2 = X2$	$b = A2$
$\lg x_3 = X3$	$t = An$

The model can be treated by a multiple linear regression:
$Y = A0 + A1*X1 + A2*X2 + A3*X3$
In order to establish what is the weight for each factor (values for the unknowns: A0, A1,…An), we must make a lot of design experiments.

CONCLUSION

It is important to know the comportment of introducing a new material in the design of product classes.
By understanding the impact that it has such equipment, project leaders can know who is carrying the weight of each factor influencing the design process and its outcome.
In addition, they will know it is team work, how to allocate resources and what tests should be made.
Proposal of a mathematical model to study the deposition process is an important step to understanding and managing them.
In order to be completed, this work must be continued by a lot of experiments, where the doped ZnO nanoparticules are involved.

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