Simulation of Process Parameters for the Growth of Ba-Doped ZnO Nano-Rods Using Fuzzy Analysis

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ABSTRACT

Advancement in technology and industrialization has made nano-technology a significant research area. Among the wider field of nano-technology, nano-materials are considered as the future of research and applications. Due to their unique properties, nano-materials are gaining enormous attention in the field of energy, medical, electronics and chemistry. These materials exhibits advanced properties and provide large surface area to volume ratio due to decrease in their rod dimeter. Between other nano-materials, ZnO (Zinc Oxide) nano-structures are extensively known due to their excellent piezo and pyro electric properties. Various materials are doped with ZnO to decrease its rod diameter for advanced application. In this work, we have fabricated, simulated and studied Barium doped ZnO nano-rods and their effect on the rod diameter using fuzzy analysis. The result depicts that the rod diameter decrease with increase in barium doping and process temperature for the growth of ZnO nano-rods. The simulated results are compared with the fabricated results and the calculated results, with less than 1% error in the value. The fabricated Ba (Barium)-doped ZnOnano-rods are highly symmetric and show hexagonal geometry. The size of the nano-rods is also similar to the Mamdani model simulated results. Ba-doped ZnO nano-rods are thus suitable for nano-scale applications including energy harvesting and bio-medical applications.

Key Words: Zinc Oxide, Nano-Rods, Fuzzy Analysis, Barium Doped ZnO.

1. INTRODUCTION

Nano technology has extensively added up to the work of research in almost every field of life directly or indirectly. The most important thing in nano materials is its novel properties which different nano material exhibits. The small size of nano materials is responsible for its every kind of practical use [1]. Specially nano materials of ZnO have attracted the scientists in this aspect because of its wide direct band gape(3.37ev) and excitation binding energy(60ev) and piezoelectric properties which make it vital for nano-electronics, optoelectronics and energy harvesting [2-3]. ZnO has remarkable specific capacitance, high chemical stability, good electrical conductivity, and fast redox kinetics [4]. It has a lot of practical applications, such as in optoelectronic devices (laser diodes, light emitting diodes, photodetectors), electronic devices (Transistors, ICs), catalysts, sensors, energy harvesting devices, active compounds in sunscreens, etc. [5-7]. A lot of research has been conducted on synthesizing one-dimensional ZnO nano-structures and on studying their morphologies according to their shape-related optical and electrical properties. Various types of ZnO nanostructures have been considered, such as, nano-rods, nano-wires, nano-tubes, nano-helixes, nano-belts, seamless nano-rings, nano-dots, mesoporous single-crystal nano-wires and polyhedral cages nano-wires and nano-rods. In all structures nano-rods and nano-wires are being studied widely because of the ease of their production and device applications [8-9]. They are used as both functional units and interlinks in the formation of optoelectronic, electronic, electrochemical and electromechanical nano-devices. ZnO is synthesized by various techniques such as thermal decomposition, laser ablation, chemical vapour deposition, precipitation, hydro-thermal, electrochemical depositions, combustion, ultrasound, thermal evaporation under vacuum ormechano-chemical-thermal synthesis. And to open up possibilities of new applications in photonics, photocatalytic, and light emitting diode devices, second group elements of periodic table are considered as good doping elements for conforming the structure and morphology of ZnO [10-12]. For example, the doping of Mg in ZnO produced significant changes in properties, it increased the photocatalytic activity [13]. Some groups synthesized Ba-doped ZnO expressing modifications in ferroelectric and catalyticproperties [14-15]. In the same way ZnO is doped by other second group elements as well. Despite, Ba has a greater ionic radius than that of ZnO, substitution is still difficult with the help of ordinary general doping rules. Among these second group elements, Ba doping is important because of its applications in varistors and liquid sensors' guiding layers [16]. But literature provides a very few reports on Ba-doped ZnO nano-rods.

Various simulations tools can be adopted which provides experimentalist the righteousness and efficiency of the design before it is actually built up. There are different ways for the simulation including ANYSY, TRANSYS and MATLAB for structural, mechanical, magnetic and parametric estimations of the material to be fabricated. Among these methods, FLC (Fuzzy Logic Controller) is highly efficient software providing a very valuable flexibility for reasoning. This is a good way to consider the inaccuracies and uncertainties of any experiment. It is a technique to impose human-like thinking into a controlled experiment.

In this paper we discuss the simulation and synthesis of growth of Ba-doped ZnO nano-rods ranged from 50-300nm rod diameter are presented according to the doping percentage and temperature. Rods of this size will improve the energy harvesting capability and can be widely used for solar energy and bio-medical applications.

2. MATERIALAND METHODS

Ba-doped ZnO nano-rods are fabricated using self-designed chemical bath deposition temperature. Zinc acetate di-hydrate is used as a precursor of ZnO and ba-acetate is used for ba-doping. Glass substrate was initially cleaned using ultra-sonication bath with DI water and acetone. The cleaned glass substrate is then subjected to seeding. Seeding layer is a thin film of ZnO nano-particles that facilitates to growth of ZnO ano-rods. 5mM zinc acetate dehydrate is dissolved in 40 ml of 2-propanol. The substrate was dipped in the solution at a rate of 20 dips per minute for 2 minutes followed by drying at 80^{O}C for 15 minute to properly evaporate the solvents. Solution of 20mm of Zinc acetate di-hydrate, hexa-methylene tetra amine and 1.3% ba-acetate was stirred in DI water. This solution is inserted in the chemical bath deposition setup. The temperature was set at 95^{o}C for 3 hours. After 3 hours the film was annealed at 470^{o}C. The doping and annealing temperature was set on the basis of fuzzy analysis performed in section 3 for the validation of results.

The prepared Ba-doped nano-rods are then characterized using scanning electron microscopy for the structural analysis of the film

3. FUZZY SYSTEM DESIGN

With the help of fuzzy analysis we have shown up the input variables, 'Ba-doping concentration in ZnO' and 'the process temperature' along with the output 'rod diameter' on fuzzy inference editor shown in Fig. 1, Because fuzzy logic provides almost ideal conditions, it has numerous values between 0 and 1.

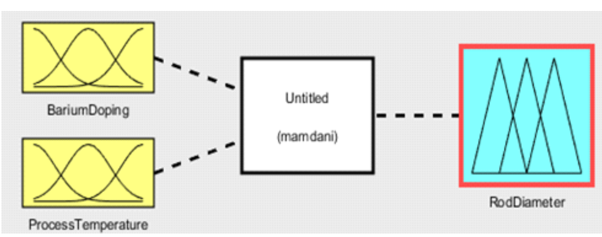

FIG. 1. FUZZY INFERENCE SYSTEM FOR THE ROD DIAMETER OF BA DOPED ZNONANO-RODS

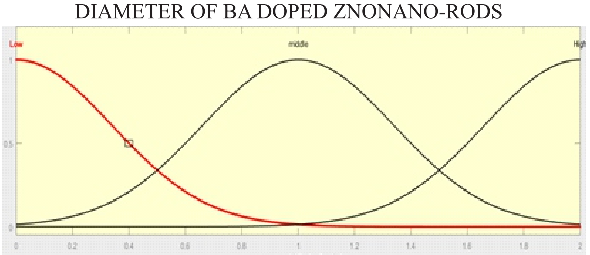

FIG. 2. MEMBERSHIP FUNCTION GRAPH SHOWING BARIUM DOPING(0-2%)

The graphs for the input and output variables have been drawn by MATLAB membership function. The graphs for the inputs, Ba-doping percentage and process temperature and output rod diameter are shown in Figs. 2-4 respectively. The input parameter of barium concentration was taken in the range of 0-2%. The range for process temperature was taken from 200-600^{o}C. The ranges for output parameter are 50-300 nm.

The rules are defined in the MATLAB rule editor using IF, AND, and THEN logic, based on the real life value. On the basis of the rules, the 2D and 3D graphs are studied. To show up the three values at a time in a graph 'two inputs and one output' we have three dimensional graph shown in Fig. 5.

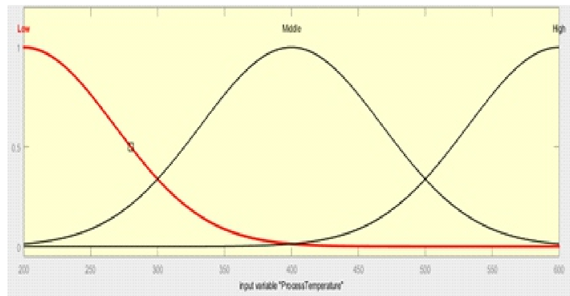

FIG. 3.MEMBERSHIP FUNCTION GRAPH SHOWING PROCESS TEMPERATURE (200-600^{o}C)

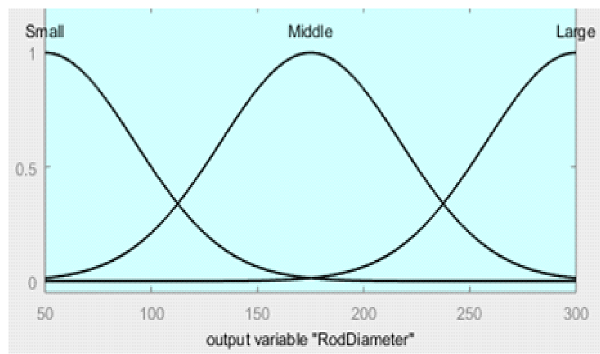

FIG. 4.MEMBERSHIP FUNCTION SHOWING ROD DIAMETER (50-300 nm)

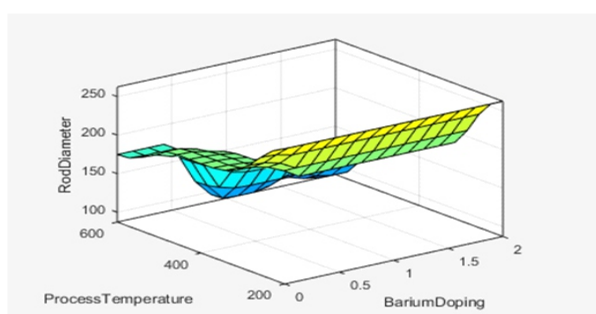

FIG. 5. THREE DIMENSIONAL GRAPH SHOWING ALL THE THREE VARIABLES

The Figs. 6-7 show the behavior of both the inputs with the output individually. Fig.6 shows the 2D graph of rod diameter and process temperature. The decrease in rod diameter with increase in temperature depicts the creation of crystals with small size. High annealing temperature will results in the change of phase of Ba-doped ZnO nano-rods which will result in decrease in diameter. These crystals can be more beneficial because they will occupy less surface area which will result in an increase in surface area to volume ratio. On the other hand shown in Fig. 7 shows the 2D graph of the two quantities rod diameter and percentage doping. Which increase in ba-doping rod diameter decrease which will result in an increase in surface area to volume ratio.

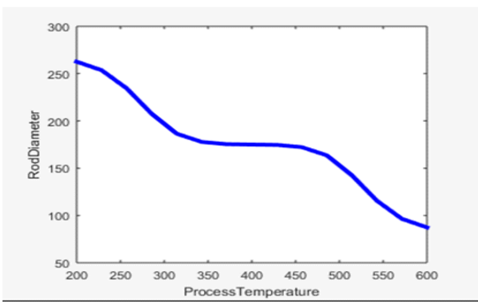

FIG. 6. 2D GRAPH BETWEEN ROD DIAMETER AND PROCESS TEMPERATURE

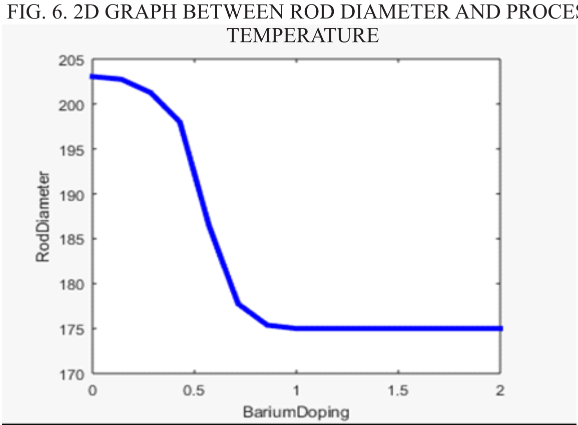

FIG. 7. 2D GRAPH OF BETWEEN ROD DIAMETER AND PERCENTAGE DOPING

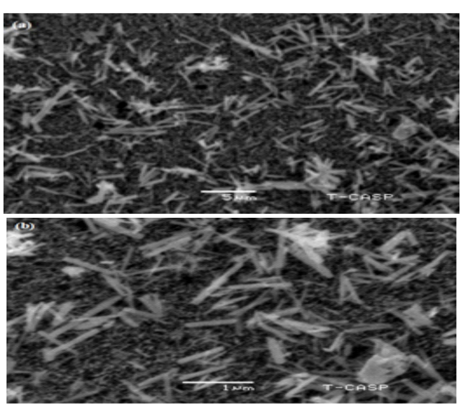

FIG. 8. SEM MICROGRAPHS OF BA-DOPED ZNO NANORODS

3. ANALYSIS AND RESULTS

The SEM (Scanning Electron Microscopy) graphs are shown in Fig. 8. These graphs show the growth of Ba-doped ZnO nano-rods. These rods are symmetric and shown in the micro-graphs and have hexagonal geometry. The average diameter of the prepared nano-rods is I range of 165-175 nm. From the rule viewer in fuzzy analysis, the crisp value of rod diameter is studied which is equal to 169 nm, which lies in the range of the average value of the rod diameter calculated using SEM. The rules defined by the rule editor are viewed in the rule viewer. For calculations, a crisp value of both inputs is selected. On the basis of these crisp values a comparison is carried out in between the simulated value of output and the calculated value (Fig. 9).

Calculation was performed for the crisp value of Ba-doping of 1.35% and process temperature of 471°C.For these corresponding crisp values the rod diameter is 169 nm. Both the input values lie in the membership function region "High". On the basis of these tow value 4 values of membership functions are calculated. These membership functions values are calculated from the selected crisp values as shown in Fig.9. These values depict the highest and the lowest value of the crisp value range. The membership function values are:

$b_1 = 2 - 1.35/2 = 0.325\%$
$b_2 = 1 - b_1 = 0.675\%$
$b_3 = 600-471/600 = 0.215^{o}C$
$b_4 = 1 - b_3 = 0.785^{o}C$

For the values of membership function 4 rules are selected out of 9 rules which are considered for this work. The minimum membership function value (Gi) and Singleton value (Vi) is calculated based on mamdani

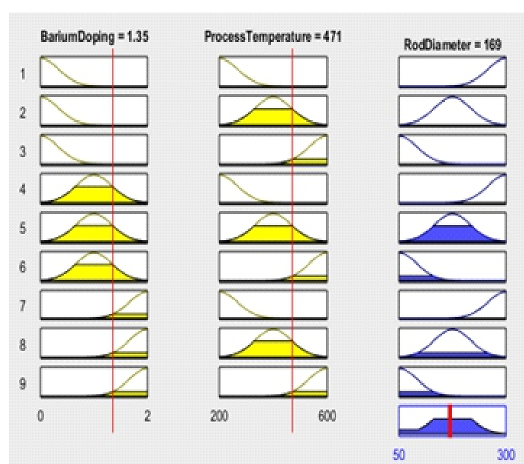

FIG. 9. RULE VIEWER' TO SHOW UP ONE OUTPUT FOR THE CORRESPONDING TWO INPUTS

formulae. The sum of all the minimum membership function values and singleton values are calculated which are furthermore used to calculate the crisp value of output using Mamdani model.

$\sum Gi = 1.43$

$\sum Gi \times Vi = 2.4$

Mamdani model = [Σ(Gi × Vi) / Gi] *100

Mamdani model = 168 nm

The Crisp value of the output from rule viewer is 169 and mamdani model calculated value is 138. The error between the simulated value and the calculated value is less than 1% which shows the accuracy of the results. These Ba-doped ZnO nano-rods based structures can be synthesized and can be used for various nano-rods diameter based nano-scale applications.

4. CONCLUSION

In this work, the effect of ba-doping on ZnO nano-rods was studied using fuzzy analysis. The results depicts that the rise in temperature and ba-doping will results a decrease in rod diameter. The decrease in rod diameter is directly attributed to the decrease in nano-rods size which will results in a large surface area to volume ratio. The fabricated ba-doped ZnO nano-rods and fuzzy analysis results show that the simulated and calculated values are similar to each other with less than 1% error in the value. The results show that barium doping will eventually results in a decrease in rods diameter which make is suitable for nano-scale applications.

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