

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Design, Simulation and Optimization Of ZnO Nanorod For Energy Harvesting Application.

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ABSTRACT

Power generation from piezoelectric materials like Zinc Oxide (ZnO) has led to many self-powered applications in the field of Nanotechnology. ZnO nanogenerator has replaced the existing power supplies for micro and nanoelectronic devices. In this proposal, the effect of ZnO nanorod's height and diameter in the overall output performance of the ZnO nanogenerator are investigated. Finite element analysis (FEA) is used for modeling the ZnO nanorod. The modeled ZnO nanorod is altered with varied height values from 900 nm to 1500 nm and diameter values from 20nm to 50 nm and is subjected to constant mechanical force of 0.95N/m². The output characteristics in terms of stress, strain and displacement due to the mechanical force given on the nanorod are observed in all the cases and analyzed. It was observed that the ZnO nanorod with 1500 nm height and 50 nm diameter provided better output characteristics with maximum deflection in terms of 14.4 nm displacement .This gives the overall view of output performance dependency on the height and diameter of the ZnO nanorod. Using this simulated optimized output, an enhanced ZnO self-powered nanogenerator can be synthesized with increased efficiency in practical case for various energy harvesting applications. **Keywords:** Energy harvester, Nanogenerator, Piezoelectric, Self-powered, ZnO



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INTRODUCTION

Energy harvesting technologies have accrued attention to replace power supplies and batteries for very small electronic devices over a decade. Energy scavenging from easily available materials using cost effective methods to provide improved efficiency, portability, easy maintenance and environmental friendly characteristics are the major challenges faced in the modeling of any energy harvester. Piezoelectric materials have both ferrro and piezoelectric properties which gives high piezoelectric response to have high performances [1].Piezoelectric materials can harvest electrical energy from the mechanical energy given in the form of vibrations and act as a desirable power source [2][3]. Piezoelectric concept originated in 1880 led to first application of piezoelectric device transducer in World War 1. Then on many researchers started working with piezoelectric nanostructures to provide a better energy scavenger or energy harvester, as acquiring electric power from the applied input in the form of mechanical force alone on the piezoelectric material is easy. Among the available piezoelectric materials such as Barium Titanate, Lithium niobate, Potassium niobate, etc., Zinc Oxide in Wurtzite structure is stable, non-toxic, crystallographically aligned [4], easily synthesizable by low temperature methods [5][6], and cost effective. Also ZnO nanostructures can provide very high efficiency under any form of mechanical stress on it [7]. Different nanostructures of Zinc Oxide like nanorod, nanorflakes, nanoflowers, nanosheets etc., can be synthesized in laboratories under ambient conditions. Experimenting multifunctional applications using Zinc Oxide such as biosensors [8], resonators [9] and electric nanogenerators [10] have already been done. But the enhancement of the output is still a major concerning issue for the current researches because of the output performances dependent factors like surface carrier density of ZnO nanostructures [11], device synthesizing methods [12][13], selection of electrodes[14][15], seed solution concentration, seed layer [16] and nanostructure growth solution[17], type of dopants added to nanostructures[18], type of junction formed like P-N junction, Schottky junction etc..Hence proper optimization of the nanostructures considering these dependency factors is recommended to have desired and enhanced output performances. Of all the ZnO nanostructures available, ZnO 1Dnanorod structure is comparatively better for efficient carrier transportation facilitation with reduced surface disorders, defects surface, discontinued interfaces[19][20].

This paper deals about the design and modeling ZnO nanorod using Finite element analyzer under stress-strain mode. Analysis is done on ZnO nanorod with varied aspect ratio to find its impact in the overall performance of energy harvester when designed practically. Stress, Strain and displacement analysis is done to have better idea about the impact created when the mechanical force is applied on the ZnO nanorods.

MATERIAL SELECTION

To have targeted output and have high beneficial applications, it is necessary to have perfect materials selected as they constitute the foundation for the fabrication of any device. Based upon the application and output expected, different materials are to be selected as different materials have their own respective properties and behaviors under different conditions. As this proposal concentrates on P-N junction formation, it is highly desirable to choose ZnO, a piezoelectric material for modeling the nanorod as it is N-type material, bio safe, biocompatible, cost effective and exhibits different nanorod structures at low temperature synthesizing methods[5][6].

SIMULATION AND RESULTS

Finite Element Analysis is used to model the nanorod. Solid mechanics and piezoelectric study is chosen to observe displacement, stress and strain effects on the nanorod. The bottom part of the designed nanorod is kept fixed by applying the fixed constraint to observe the nanorod bend or deformation in the form of displacement when a mechanical force of 0.95N/m² in the form of boundary load is applied in the upper part of designed ZnO nanorod. The height and diameter of the ZnO nanorod are varied from 900-1500 nm and 20-50 nm respectively. Selection of type of mesh with its relevant parametric adjustments are more important to have a more accurate solution. There are many forms of meshes available. Out of those, tetrahedral meshing is selected as it can be used to any shape or topology with any 3D volume for testing. Also the output characteristics can be more accurately measured using this type of mesh as the device consists of thin layers. In all the mentioned cases, same mechanical force in the form of boundary load is applied. Respective stress, strain and displacement analysis were obtained and tabulated.

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2017(Suppl.)

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Figure 1 gives the displacement, stress and strain values obtained under mechanical force of 0.95N/m².These gives the range of values for displacement, stress and strain obtained in terms of color variations. The red and dark blue color in the figure 1 denotes the highest and lowest value respectively for displacements, stress and strain obtained. From the table 1 output analysis, it is observed that when the height and breadth of the nanorod is increased, the stress and displacement value also increases with decrease in strain value. So, when the total area of the rod is increased, maximum stress encountered by the nanorod with high deflection in the form of displacement is observed. When there is maximum deflection produced, the nanorod will yield higher output voltage signals as reported by Wang et al experiment [9]. From these observations, it is clear that height and breadth of ZnO nanorod has greater influence in the output performances of a ZnO energy harvester device. Therefore it is evident that aspect ratio influence also plays greater part in obtaining a better performance nanogenerator.



Figure 1- A FEA result of ZnO nanorod (i) Displacement obtained (ii) Stress obtained (iii) Strain obtained.

Diameter (nm)	Height (nm)	Displacement (nm)	Stress (N/m²)	Strain
20	900	2.81	1.92X10 ⁹	0.18X10 ⁻³
50	900	4.82	2.09X10 ⁹	0.14X10 ⁻³
20	1200	6.81	3.88X10 ⁹	0.11X10 ⁻³
50	1500	9.02	5.82X10 ⁹	0.09X10 ⁻³
20	1500	12.85	6.02X10 ⁹	0.07X10 ⁻³
50	1500	14.4	8.23X10 ⁹	0.04X10 ⁻³

Table 1: ZnO nanorod's FEA output

CONCLUSIONS

The effect of ZnO nanorod's height and diameter in the overall output performance of the ZnO selfpowered nanogenerator is investigated using Finite Element Analysis tool. Varying the height and diameter of ZnO nanorod under same mechanical force of 0.95 N/m² is carried out. It is evident that the rod with 1500 nm and 50nm of height and diameter respectively provided higher deflection of 14.4 nm with stress and strain values of 8.23X10⁹N/m² and 0.04X10⁻³ respectively. The ZnO nanorod with more deflection has yielded higher output. Therefore, it is clear that ZnO nanorod's diameter and height optimization is highly necessary to have a desired output performances. Thus, using the simulated results, it is beneficial to grow ZnO nanorod at laboratories using low temperature methods like hydrothermal, chemical vapor deposition methods with the dimensions optimized here so as to obtain an enhanced output to have a better performance energy harvester for varied applications. By exposing the fabricated device practically to the desired gas under ambient conditions, it can be made to work as a gas sensor also.

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