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Electrical energy generation from nanowire structures

R. R. Attab C. A. Emshary

Physics Department-College of Education for Pure Science- Basrah University

Abstract

This work numerically estimate the amount of electric voltage generation from Zing oxide, Barium titanium, Gallium nitride, Lead zirconate titanate (ZnO, $BaTiO_3$, GaN and PZT) nanowire structure respectively and other hetro-structure or doped structure like (ZnMgO, GaAlN) having rectangular and circular cross sections with dimension of length and width (l , b) 600,50 nanometers. The amount of the generated voltage seem enough to power biosensor, nanosensor, or even biomedical device. The effect of nanowire length, width and temperature and the effect of applied force are studied, All theses parameters having profound effect on the amount of the maximum generated voltage.

توليد الطاقة الكهربائية من تراكيب الاسلاك النانوية

رسول رمضان عتاب جاسب عبد الحسين مشاري

قسم الفيزياء- كلية التربية للعلوم الصرفة- جامعة البصرة

الخلاصة

في هذا العمل تم تقدير كمية الفولتية الكهربائية المستحصلة من المواد (PZT, ZnMgO, GaAlN) ZnO, $BaTiO_3$, GaN عددياً والتي تكون على شكل تراكيب اسلاك نانوية ذات مقاطع مستطيلة ودائرية. ان مقدار الفولتية المتولدة كافية لتشغيل اجهزة ذات قدرة قليلة كأن تكون على شكل متحسسات حياتية، متحسسات نانوية، اجهزة طبية. ان تاثير خواص السلك النانوي مثل الطول والعرض ودرجة الحرارة وكذلك اثر القوة المسلطة قد درست جميعا. بدا ان لكافة المعاملات المذكورة اثر واضح في مقدار الفولتية العظمى المتولدة.

Introduction

With the threatening of global warming and energy crises, searching for renewable and green energy resources is one of the most urgent challenges to sustainable development of human civilization. At the large-scale, besides the well known energy resources that powered the world today, such as petroleum, coal, hydraulic, natural gas and nuclear, active research and development are being taken in exploring alternative energy resources such as solar, geothermal, biomass, nuclear, wind, and hydrogen. At a much smaller scale, energy and technologies are desperately needed for independent, sustainable, maintain-free and continuous operations of implantable biosensors, ultrasensitive chemical and bio-molecular sensors, nano-robot, micro-electromechanical systems, remote and mobile environmental sensors, homeland security and even portable wearable personal electronics [1-3]. Building self-power nanosystems is a future direction of nanotechnology [4]. A nanosystem is an integration of nanodevices, functional components, and a power source. Energy harvesting from the environment for powering a nanosystem is vitally important for its independent, wireless and sustainable operation [5]. A piezoelectric nanogenerator (NG) is a promising approach for this application. The NG is based on a vertically aligned ZnO (for example) nanowire (NW) array that is placed beneath a zigzag electrode with a small gap [6]. The NG relies on the piezoelectric potential created in a nanowire once subjected to elastic straining, which drives the flow of charge carriers [7].

The zigzag electrode acts as an array of parallel integrated tips for simultaneously creating, collecting and outputting electricity from all of the active NWs. In this paper we present the results of calculating the maximum harvested voltage from Zing oxide, Barium titanium, Gallium nitride, Lead zirconate titanate (ZnO, $BaTiO_3$, GaN and PZT) nanowire structure respectively and other hetro-structure or doped structure like (ZnMgO, GaAlN) in the form of nanowires of two different cross-sections viz rectangular and circular as functions of NW length, width, temperature and applied force.

Basic model

To derive a theoretical expression for the harvested voltage from a NW, for a dielectric and piezoelectric material system, when the material is placed in an electric field and subjected to an external force Fy, the constitutive equations are[7]:

$$\sigma_{ij}=c_{ijkl}\epsilon_{kl}-e_{ijk}E_k-\alpha_{ij}\Delta t \quad (1)$$

$$D_i=e_{ijk}\epsilon_{ik}+\varepsilon_{ij}E_i+p_i\Delta t \quad (2)$$

Here, the mechanical stress tensor σij and mechanical strain tensor ϵ_{ik} , The dielectric displacement Di and the electric field Ei and the temperature change Δt , e_{ijk} , ε_{ij} , c_{ijkl} are the linear piezoelectric coefficient, dielectric constant and elastic constant respectively. α_{ij} , p_i are the thermoelastic and pyroelectric coefficients respectively.

1- Rectangular NW structure

When a lateral force Fy is applied at the free end of the NW and parallel to y-direction (see Figure1), normal stress σzz and shear stress components σxz and σyz appeared on the cross section along the z-direction, while other three components σzz , σxz and σyz are zero. Based on the saint- venant cantilever bending theory for a rectangular beam [8], one can calculate mathematical expression for σzz , σxy and σxz [8]. By the same way one can find expression for the strain components and the electric displacement. When a constant external voltage v_y is applied on the NW along the y-direction and a uniform electric field $E_y=\frac{v_y}{b}$ will be induced inside the nanowire, and for a general case that both Fy and v_y present.

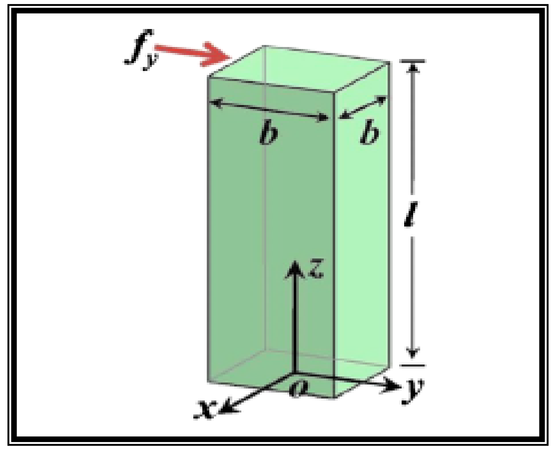


Figure (1): The rectangular cross section nanowire with external force F_y [9].

To find out the total or maximum harvested voltage one can write down a general expression for the total energy stored in the NW (U_{tot} (volt)).The total charge Q_{tot} on the two side surfaces of the NW can be written as[10]:

$$Q_{tot}=\frac{\partial U_{tot}}{\partial v_y} \quad (3)$$

$$Q=\left[\frac{F_y(1+\nu)e_{15}lb^3}{96EI_{xx}}+2\left(\frac{(1+\nu)}{2E}e_{15}{}^2+\frac{1}{4}k_{11}\right)lv_y\right]-\left(\frac{(1+\nu)e_{15}}{2E}\alpha_{xz}\Delta t-\frac{1}{4}p_{xz}\Delta t\right)bl \quad (4)$$

where E – young modulus, ν - poisson ratio, I_{xx} - moment of inertia, α_{xz}, p_{xz} are the thermoelastic coefficient and pyroelectric coefficient respectively. e_{15}, k_{11} are piezoelectric and dielectric constants. Hence the NWs capacitance C_p along the y-direction is:

$$C_p=\frac{\partial Q}{\partial v_y}=2\left[\frac{(1+\nu)}{2E}e_{15}^2+\frac{1}{4}k_{11}\right]l \quad (5)$$

The total harvested voltage Δv_{max} is:

$$\Delta v_{max}=\frac{\left[\frac{F_y(1+\nu)e_{15}lb^3}{96EI_{xx}}+2\left(\frac{(1+\nu)}{2E}e_{15}{}^2+\frac{1}{4}k_{11}\right)lv_y\right]-\left(\frac{(1+\nu)e_{15}}{2E}\alpha_{xz}\Delta t-\frac{1}{4}p_{xz}\Delta t\right)bl}{2\left[\frac{(1+\nu)}{2E}e_{15}^2+\frac{1}{4}k_{11}\right]l} \quad (6)$$

Here the term that associated with temperature variance (Δt) is:

$$\left(\frac{(1+\nu)e_{15}}{E}\alpha_{xz}\Delta t-\frac{1}{2}p_{xz}\Delta t\right)$$

In many applications for piezoelectric NW generators no applied voltage is present and the NW is considered as an open circuit system thus eq.(6) can be reduced to :

$$\Delta v_{max} = \frac{\left[\frac{F_y(1+v)e_{15}b^3}{96EI_{xx}}\right] - \left(\frac{(1+v)e_{15}}{E}\alpha_{xz}\Delta t - \frac{1}{4}p_{xz}\Delta t\right)b}{\left[\frac{1}{G}e_{15}^2 + \frac{1}{2}k_{11}\right]} \quad (7)$$

Where G – shear modulus.

2- Circular NW structure

Based on the figure (2) one can arrive at the final expression for the maximum harvested voltage for the circular NW:

$$\Delta v_{max} = \frac{\left[\left(\frac{3}{4}+\frac{v}{2}\right)\frac{F_y e_{15} l r^3}{12EI_{xx}}\right] + \left(\frac{(1+v)e_{15}}{E}\alpha_{xz}\Delta t - \frac{1}{2}p_{xz}\Delta t\right)rl}{2\left[\frac{(1+v)}{E}e_{15}^2 + \frac{1}{2}k_{11}\right]l} \quad (8)$$

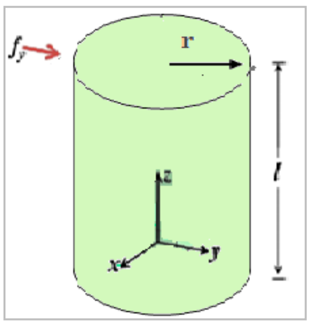


Figure (2): The circular cross section nanowire with external force[11].

Results and discussion

The maximum harvested voltage from nanowire dependence on length, width temperature and applied force. Relations are found using the equations (6) and (7) for the rectangular and circular NW for the different materials (ZnO, PZT, BaTiO3, ZNMgO, GaAlN and GaN). The pyroelectric and thermoelastic coefficients for the studied materials are given in tables 1-3. Figures (3) and (4) shows the relation between maximum voltage harvested from the NWs for both rectangular and circular shapes for the different materials, against applied force. The relations show direct proportionality of Δv_{max}(voltage) vs Fy (Newton). Figures (5) and (6) show the relation between Δv_{max} against NW length for both the rectangular and circular shapes. No clear effect of the NW length on the maximum harvested voltage.

Table (1) Pyroelectric and thermoelastic coefficients for studied materials.

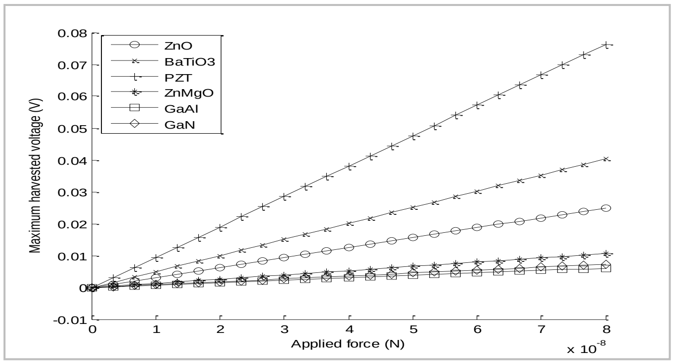
Material	Symbol	Pyroelectric coefficient $*10^{-6}$ C/m²K	Thermal expansion coefficient $*10^{-6}$ 1/mK	Reference
Lead zirconate titanate	$PbZrTiO_3$	238	6.6	12,13
Barium titanium	$BaTiO_3$	200	3.8	14
Gallium nitride	GaN	29	3.34	15,16
Zing oxide	ZnO	57	4.7	17
Hetrostruc-ture	GaAlN	121	5.59	17
Hetrostruc-ture	ZnMgO	43	13.6	17

Table (2) Compliance parameters and dielectric coefficient for studied materials.

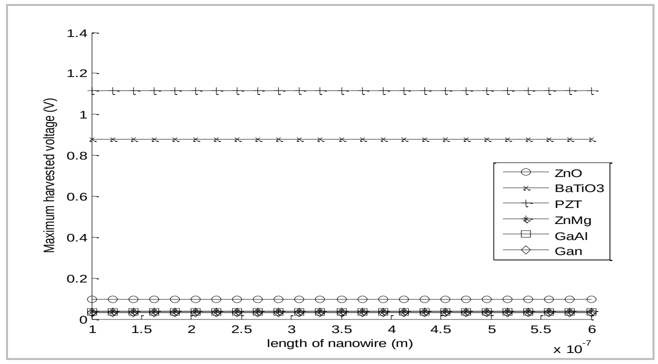
Material	K11	$C_{11}*10^9$	$C_{12}*10^9$	$C_{13}*10^9$	$C_{33}*10^9$	$C_{44}*10^9$	Reference
PZT	1800	126	79.5	84.1	117	23	18,19
$BaTiO_3$	4400	22.2	13.4	6.1	24	43	18,20
GaN	9.28	296	130	120	395	241	17,20
ZnO	7.77	207	117.7	106.1	209.5	44.8	17
GaAlN	8.5	367	135	103	405	95	17
ZnMgO	6.6	396	137	108	373	116	17

Material	e_{15} C/m²	e_{31} C/m²	e_{33} C/m²	Reference
PZT	-0.977	-1.8	9.05	21
$BaTiO_3$	-0.56	-0.7	6.7	20
GaN	-0.48	-0.6	1.46	15
ZnO	-0.45	-0.51	1.22	17
GaAlN	-0.30	-0.49	0.73	17
ZnMgO	-0.37	-0.62	0.69	17

The relations between the maximum harvested voltage and NW width are shown in Figures (7) and (8) for the two different shapes. An indirect proportionality appears i.e the increase in width leads to the reduction of Δv_{max} . The temperature dependence of Δv_{max} can be seen in figure (9) for the rectangular cross section and Figure (10) for circular one. Direct comparison between Δv_{max} against F_y for both section in ZnO NW is shown in figure (11) while the depends of Δv_{max} in ZnO for the rectangular cross section NW on applied force, F_y, length, width and temperature are shown respectively in figures (12), (13), (14) and (15).



Figure(3): The maximum harvested voltage from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN for rectangular cross section for variance nanowires against applied force.



Figure(6): The maximum harvested voltage from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN for circular cross section with length of nanowire.

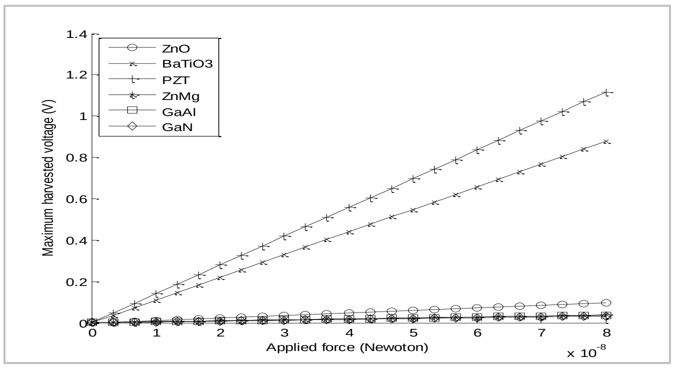


Figure (4): The maximum harvested from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN voltage for circular cross section against applied force.

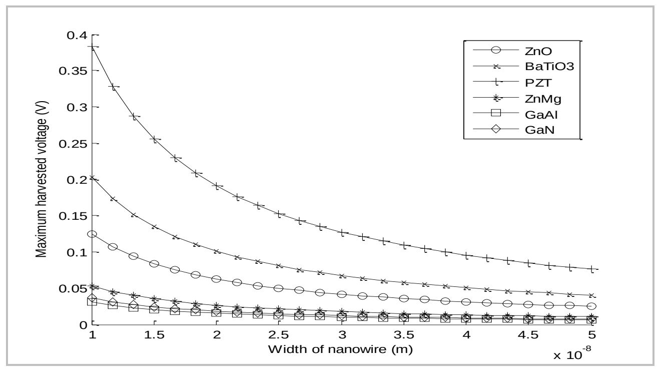


Figure (7): The maximum harvested voltage from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN for rectangular cross section against width of nanowire.

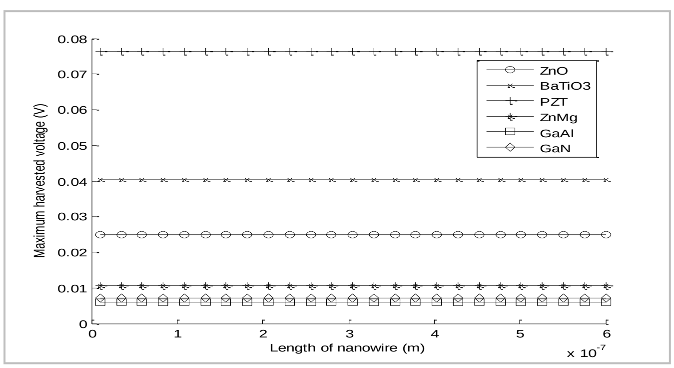


Figure (5): The maximum harvested voltage from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN for rectangular cross section against length of nanowire.

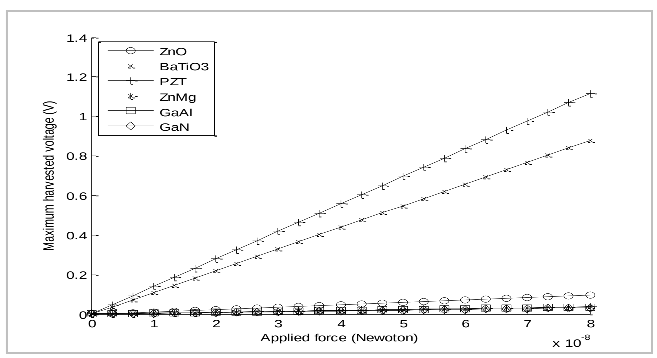


Figure (8): The maximum harvested voltage from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN for circular cross section against applied force variance.

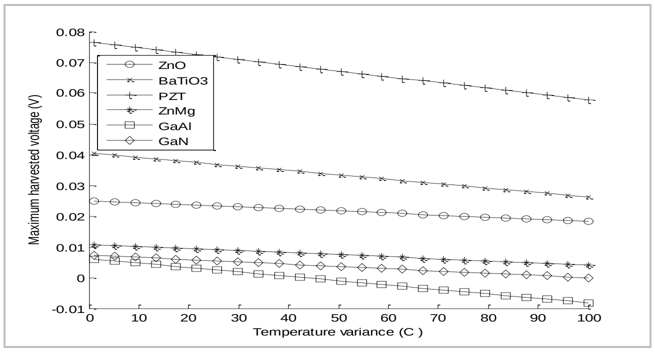


Figure (9): The maximum harvested voltage from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN for rectangular cross section against temperature variance.

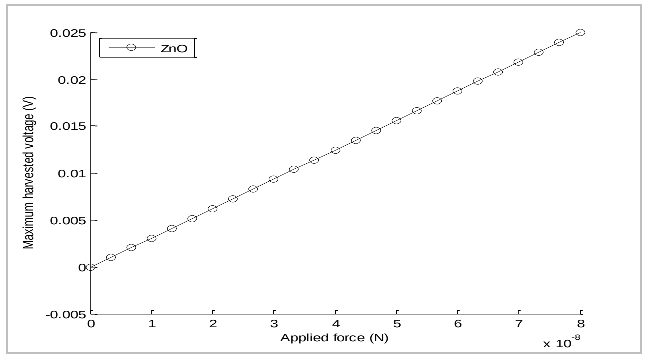


Figure (12): The maximum harvested voltage for rectangular cross section of ZnO nanowire against applied force.

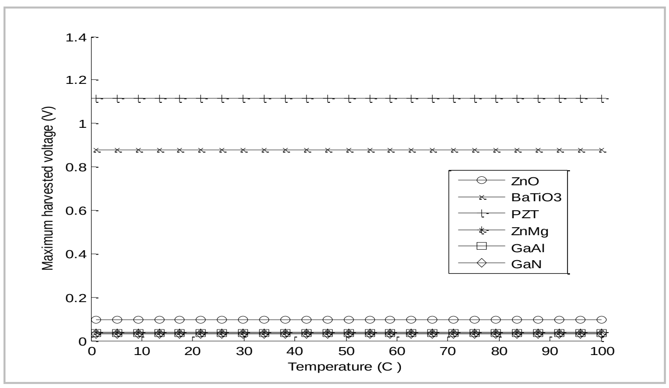


Figure (10): The maximum harvested voltage from ZnO, $BaTiO_3$, GaN, PZT, ZnMgO and GaAlN for circular cross section against temperature variance.

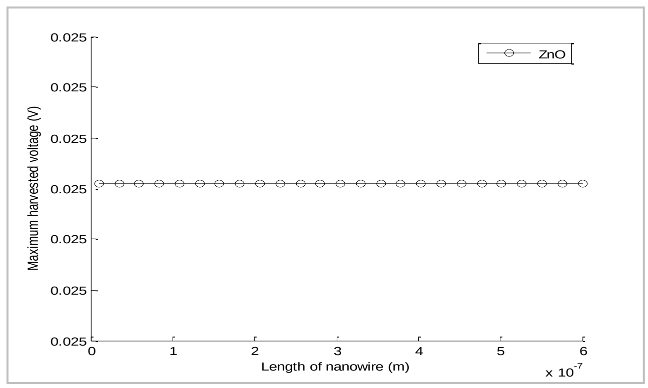


Figure (13): The maximum harvested voltage for rectangular cross section of ZnO nanowire against length of nanowire.

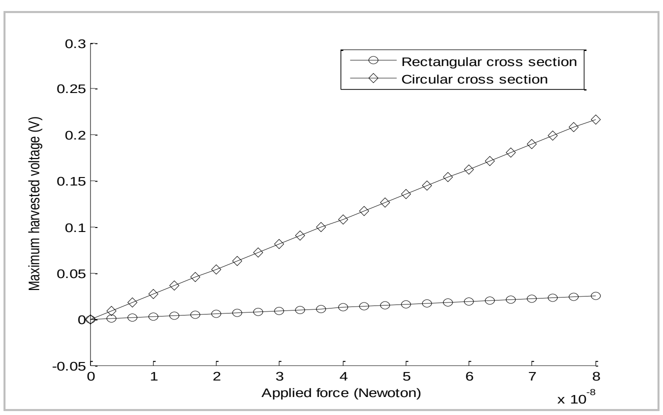


Figure (11): The maximum harvested voltage for rectangular and circular cross section of ZnO nanowire against applied force.

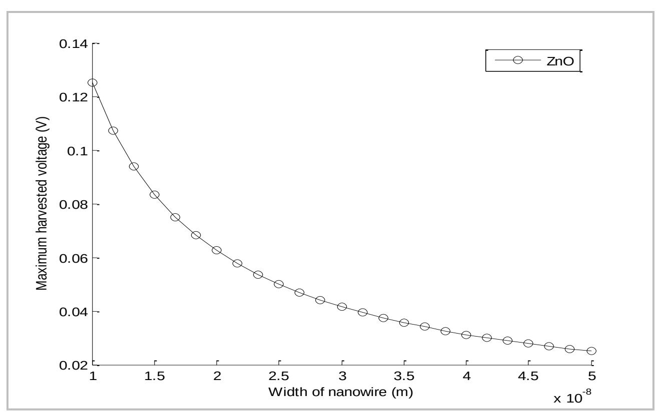
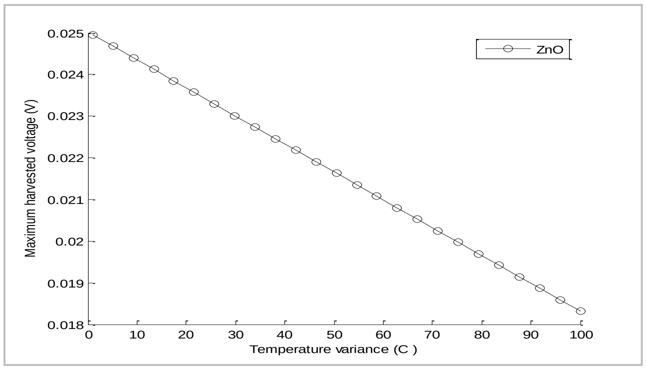


Figure (14): The maximum harvested voltage for rectangular cross section of ZnO nanowire against width of the nanowire.



Figure(15): The maximum harvested voltage for rectangular cross section of ZnO nanowire against temperature variance.

The effect of temperature on the harvested voltage from a bending nanowire by an external force F_y is proportional with the term in eqs.(6), (8) that containing the pyroelectric coefficient and the thermoelastic coefficient. The increase in temperature will produce an increase in the dimensions of the nanowire which leads to the reducution of the maximum harvested voltage. In addition to the thermoelastic behavior for the NW, the pyroelectric coefficient play an important role in energy harvesting principle because most of the studied materials having a strong pyroelectric coefficient like 4400 for $BaTiO_3$ and 1800 for PZT (see table (1), (2)). In general most of the parameters that associated with piezoelectric phenomena having a correlative relation with temperature variance due to the materials thermal, mechanical and electrical properties. The results given in this analysis indicates that nanostructures such as those previously mentioned are able to generate enough electric energy to power variance nanosystems. All parameters of the NW such as length, width, and temperature plus the applied force on the nanowire seem to have clear effects on the generated and harvested voltage.

Conclusion

In summary, we have studied the possibility of electrical energy generation from (ZnO, BaTiO3,PZT,ZnMgO, GaAlN and GaN) nanowire structure having rectangular and circular cross-section using certain theoretical calculation method. The maximum voltage obtained is enough to power nanosystem such as sensors. the maximum voltage generated seem to be effected by nanowire length, width, and temperature even with applied force to the NW.

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