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The effect of temperature on the mechanical properties of ZnO material: the calculation of generated electrical energy from ZnO nanowires

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Abstract:

This work report on the calculations of the temperature dependence of young's modulus, dielectric, piezoelectric and elastic coefficients, poisson ratio and moment of inertia. These parameters are key parameters in the calculation of electrical energy generated from bending of ZnO nanowires (NW's) of length and width equals to 600nm and 50nm respectively due to applying an external force in one direction by an AFM tip (Atomic force microscopy) in the limits of elasticity. Results show that the young's modulus and dielectric coefficient show indirect proportionality with temperature while other parameters shows direct proportionality. These parameters having profound effect on the amount of the maximum generated voltage. The effect of the dependence of young modulus on temperature on the harvested electrical energy from ZnO nanowire formed on a substrate is minor.

Key Word s: Nanowires , ZnO Nws , Electrical energy generation

1- Introduction

Smart structures based on piezoelectric materials are now finding applications in a wide variety of environmental conditions. In general, in applications, these materials or structures work at room temperatures or on a relatively narrow temperatures interval around the ambient. But there are also many applications where they have to work at temperatures above or below the ambient. Therefore, it becomes compulsory to know the behavior of their main parameters with temperature in order to make the proper design for any specific application.

However, in many applications, a transducer (or nanowire generator) having material properties and in order to predict the transducer response as a function of temperature one can estimate that response. The basic principle of electric energy generation from environment vibrations or human body movement or even sound waves by so called piezoelectric materials or structures is built on the (constitutive equations). To establish the constitutive equations between the different measurable variables of a nanowire, a set of independent and dependent variables must be chosen[1]. These variables are classified as follows:

1- Dependent variables are stress, electric displacement and entropy.
2- Independent variables are strain, electric field and temperature.

The relation between different measurable quantities of nanowire defines the material properties, The relation between stress and strain defines the stiffness or compliance, the relation between the electric field and the electric displacement defines the electric permittivity and the relation between entropy and temperature defines the heat capacities. In a piezoelectric material, these relations exist between the different electrical and mechanical domains. When introducing the thermal effects into the nanowire, the thermal domain relates both to the electrical and mechanical domain, and the material properties are not independent of each other. In this work we will show the dependence of young modulus, dielectric, piezoelectric, stiffness and elastic constants, moment of inertia, and poisson ratio on temperature since these parameters are key parameters that affect the amount of electric energy harvested from nanowire structures.

2- Theoretical part

It is known that young modulus, E, is a mathematical description of an object or substance tendency to be deformed elastically. The dependence of E on temperature can be written as [2,3]:

$$E = E_o + \frac{t\,E_o}{t_m \ln\left(\frac{t}{t_a}\right)} \qquad (1)$$

Where E_o is the young modulus at 0 K, t is the absolute temperature, t_a is the melting point, and t_m is a parameter related to the material which is suggested to have a correlation with Deby temperature Θ which is related to the volume thermal expansion and the specific heat[4,5].

Dielectric, piezoelectric and elastic constants can be calculated using the following set of equations of stress σ_{ij}, electric displacement D_i and entropy η in which reads[6,7]:

$$\sigma_{ij} = c_{ijkl}\epsilon_{kl} - e_{ijk}E_k - \alpha_{ij}\Delta t \qquad (2)$$

$$D_i = e_{ijk}\epsilon_{ik} + \varepsilon_{ij}E_i + p_i\Delta t \qquad (3)$$

$$\eta = \alpha_{ij}\epsilon_{ik} + p_iE_i + \frac{\rho C_v}{t}p_i\Delta t \qquad (4)$$

where Δt is the change in temperature, c_{ijkl} is the modulus of elasticity (N/m^2), e_{ijk} is the piezoelectric coupling (N/Vm), ε_{ij} is the permittivity of the medium (C/Vm), α_{ij} is the thermoelastic stress constants (N/m^2K), p_i is the pyroelectric constant (C/m^2K), ρC_v is the volumetric specific heat capacity (ρ is the density) (J/m^3K), E_i is the electric field (V/m), ϵ_{ik} is the mechanical strain, and t is the temperature. By differentiating the set of equations (2-4) with the respect to each components keeping the rest constant, we reach at the following equations[8]:

$$d\sigma_{ij} = \left(\frac{\partial\sigma_{ij}}{\partial\epsilon_{kl}}\right)^{E,t} d\epsilon_{kl} + \left(\frac{\partial\sigma_{ij}}{\partial E_k}\right)^{\sigma,t} dE_k + \left(\frac{\partial\sigma_{ij}}{\partial t}\right)^{\sigma,t} dt \qquad (5)$$

$$dD_i = \left(\frac{\partial D_i}{\partial \sigma_{jk}}\right)^{E,t} d\epsilon_{jk} + \left(\frac{\partial D_i}{\partial E_j}\right)^{\sigma,t} dE_j + \left(\frac{\partial D_i}{\partial t}\right)^{\sigma,t} dt \qquad (6)$$

$$d\eta = \left(\frac{\partial \eta}{\partial \sigma_{ij}}\right)^{E,t} d\epsilon_{ij} + \left(\frac{\partial \eta}{\partial E_i}\right)^{\sigma,t} dE_i + \left(\frac{\partial \eta}{\partial t}\right)^{\sigma,t} dt \qquad (7)$$

superscripts indicates the components that was held constants.

By comparing equation (5) with equations (2) and (3) we reach at the following equations[8]:

$$c_{ijkl} = \left(\frac{\partial \sigma_{ij}}{\partial \epsilon_{kl}}\right)^{E,t} \qquad (8-a)$$

$$e_{ijk} = -\left(\frac{\partial \sigma_{ij}}{\partial E_k}\right)^{\sigma,t} \qquad (8-b)$$

$$e_{ijk} = -\left(\frac{\partial \sigma_{ij}}{\partial E_k}\right)^{\sigma,t} \qquad (8-c)$$

According to the second law of thermodynamics, for a reversible change [7-9]:

$$dQ = td\eta \qquad (9)$$

where dQ is the heat flow. Substituting equation (4) in equation (9) we get:

$$dQ = td\eta = t\alpha_{ij}d\sigma_{ij} + tp_i dE_i + \rho C_v dt \qquad (10)$$

To find the adiabatic constants ($c_{ijkl}, \epsilon_{kl}, e_{ijk}, \alpha_{ij}$) the heat flow must equal to zero i.e $dQ = 0$. By solving equation (10) with this assumption we get:

$$dt = \frac{-t\alpha_{ij}d\sigma_{ij}}{\rho C_v} - \frac{tp_i dE_i}{\rho C_v} \qquad (11)$$

With the help of mathematical manipulation we arrive at the following equation that describe the adiabatic stiffness constant[8,10].

$$c^{\eta}_{ijkl} = c^{t,E}_{ijkl} + \left(\frac{t\alpha_{ij}\,\alpha_{kl}}{\rho C_v}\right) \qquad (12)$$

By following the same procedure we arrive at the following equation that describe the adiabatic piezoelectric stress constants i.e

$$e^{\eta}_{ijkl} = e^{t}_{ijkl} - \left(\frac{t\alpha_{ij}\,p_k}{\rho C_v}\right) \qquad (13)$$

And the equation that describe the adiabatic dielectric constant reads[8,10]:

$$\varepsilon^{\eta}_{ijkl} = \varepsilon^{t}_{ijkl} - \left(\frac{tp_i\,\,p_j}{\rho C_v}\right) \qquad (14)$$

The moment of inertia, I for the nanowire around the x-axis (see figure(1)) can be written as[11]:

$$I_{xx} = \frac{bl^3}{12} \qquad (15)$$

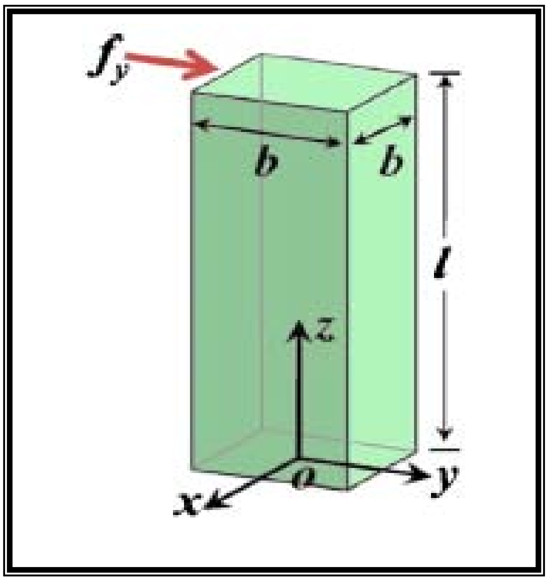
Where b and l are the width and length of the nanowire respectively. Using the following definitions:

$$\Delta l = \alpha l \Delta t \qquad (16)$$

$$b = b_o(\alpha\Delta t + 1) \qquad (17)$$

Where α is the thermal expansion coefficient, b_o is the initial nanowire width and Δl is the change in the nanowire length, we obtain

$$I_{xx} = \frac{(b_o(\alpha\Delta t + 1))^4}{12} \qquad (18)$$



Figure(1): The rectangular cross section nanowire with external force F_y [7].

Poisson ratio, ν, and its dependence on temperature can be written as follows[2]:

$$\nu = \nu_o + 3.87 * 10^{-7} t \quad (19)$$

Where ν_o is poisson ratio at room temperature.

3- Results

Since ZnO nanowires are used extensively as nanosensors, in biomedical applications, electrical energy harvesting, ect. and since (E, c_{ijkl}, ϵ_{kl}, e_{ijk}, α_{ij}, I_{xx} , ν) depends on the temperature of the nanowire so that any increment variation in temperature affect the amount of electrical energy harvested as a result of bending mechanism which is responsible for electrical energy production. The equation that describe the electrical energy harvested from a ZnO nanowire with the dimension shown in figure(1) can be written for a nanowire with a rectangular cross section as[7]:

$$\Delta v_{max} = \frac{\left[\frac{F_y(1+\nu)e_{15} l b^3}{96 E I_{xx}}\right] - \left(\frac{(1+\nu)e_{15}}{E}\alpha_{xz}\Delta t - \frac{1}{4}p_{xz}\Delta t\right) bl}{2\left[\frac{(1+\nu)}{E}e_{15}^2 + \frac{1}{4}\varepsilon_{11}\right] l} \quad (20)$$

Where F_y is the force applied to the nanowire for the sake of bending, $e_{15} = e_{ijk}$ [3], $\alpha_{xz} = \alpha_{ij}$, $p_{xz} = p_i$ and $\varepsilon_{11} = \varepsilon_{kl}$

The ZnO nanowire is formed on a substrate made of (in most applications) of silicon (Si) to meet the condition of lattice mismatch condition to form the energy levels for electron generation[12].

3-1 Temperature effect on young modulus

To show the effect of temperature on young modulus we have solved equation (1) using the following equations to find out the Young modulus at 0 K as [7]:

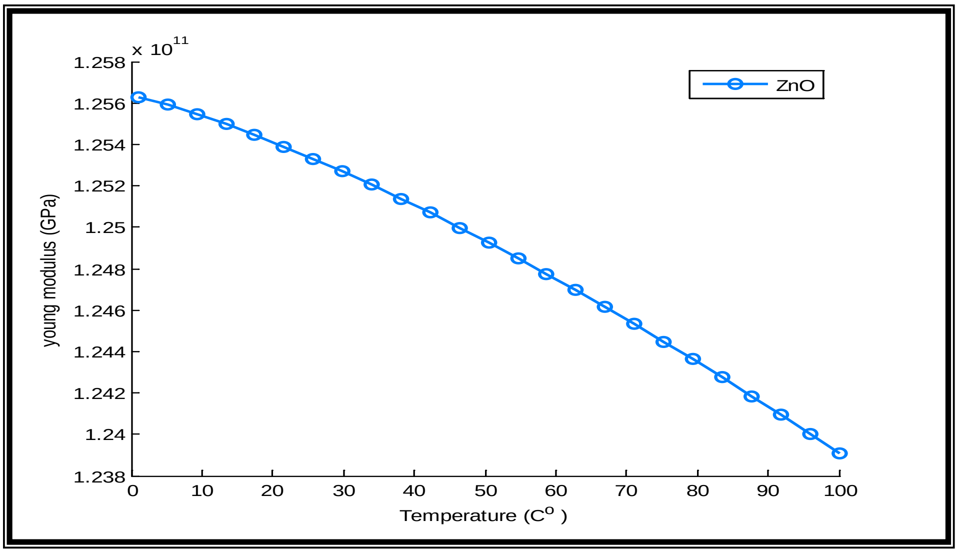
$$E_o = \frac{(A - B + 3C)(A + 2B)}{2A + 3B + C} \quad (21)$$

$$A = \frac{2c_{11} + c_{33}}{3} \quad (22.a)$$

$$B = \frac{2c_{13} + c_{12}}{3} \quad (22.b)$$

$$C = \frac{2c_{44} + c_{66}}{3} \quad (22.c)$$

And the constants are (C_{11}=207 ,C_{12}=117.7, C_{13}=106.1, C_{33}=209.5, C_{44}=44.8, C_{66}=44.29), t_m =2248 C^o, t_a =1976 C^o , ρC_v=40.3 J/(mol* K) [9]. The constants C_{ij} are calculated according to equation(12) since they are temperature dependent too. Figure (2) shows the young modulus dependence on temperature.

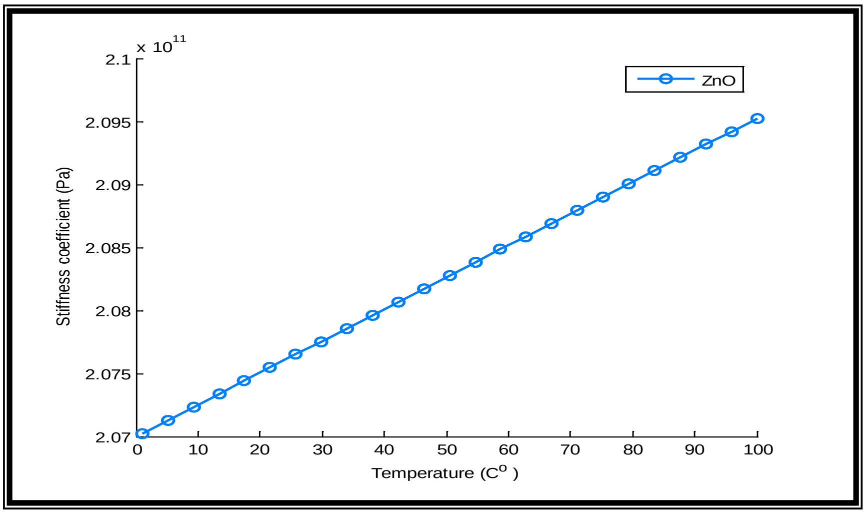


Figure(2): The dependence of young modulus on temperature for ZnO nanowire.

According to the results shown in figure (2) young modulus decreases with the increase in temperature.

3-2 Temperature effect on stiffness coefficient

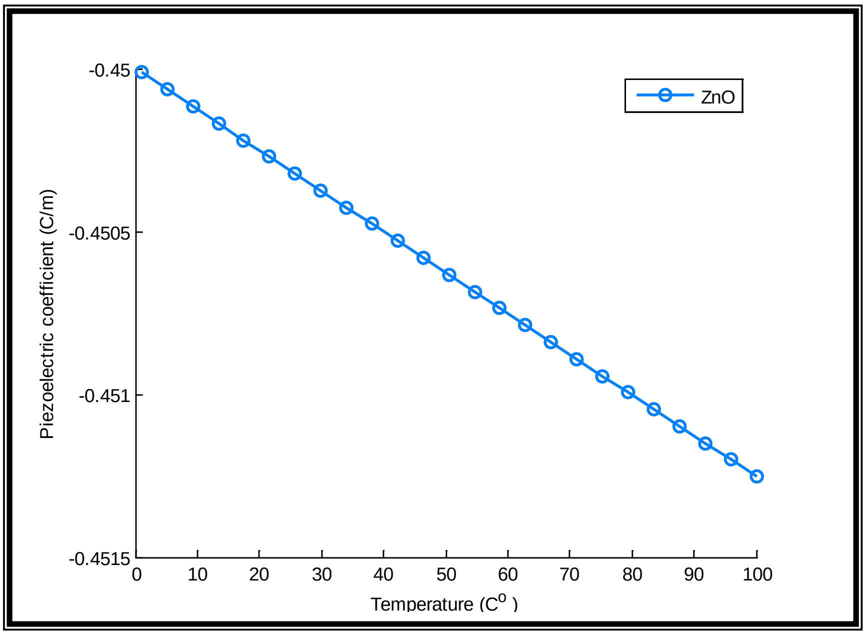
To show the effect of temperature on stiffness coefficient we solve equation (12) using the required constants as thermal expansion coefficient (4.7*10^{-6} 1/m^{2}K) and pyroelectric coefficient (57*10^{-6} C/m^{2}K) the result is shown in figure (3). The stiffness coefficient is directly related to the temperature.



Figure(3): The dependence of stiffness coefficient on temperature for ZnO nanowire.

3-3 Temperature effect on piezoelectric coefficient

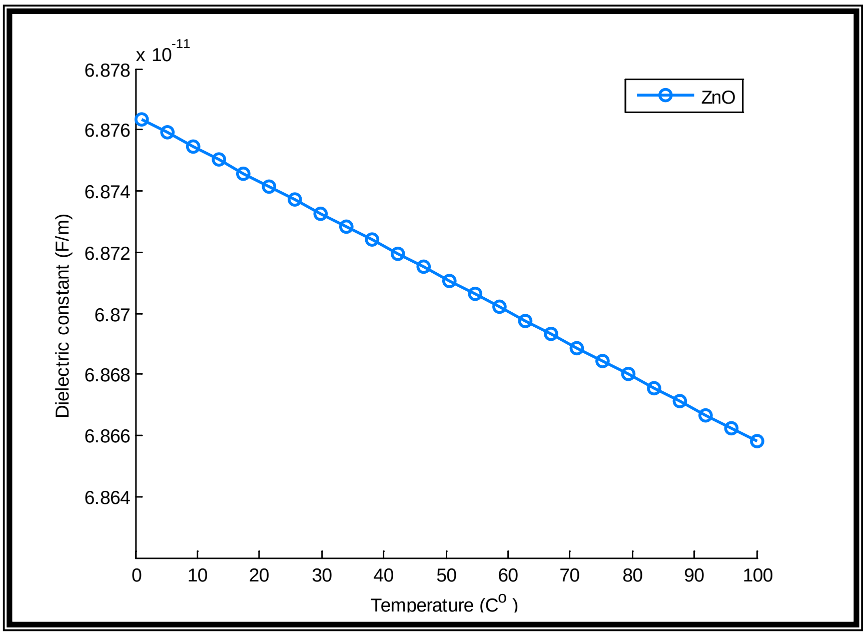
To show the effect of temperature on piezoelectric coefficient we solve equation (13) using the required constant of the piezoelectric coefficient at room temperature ($e_{ijk} = e_{15} = -0.45\ C/m^2$) , the result is shown in figure (4). The piezoelectric coefficient is inversely related to the temperature.



Figure(4): The dependence of piezoelectric coefficient on temperature for ZnO nanowire.

3-4 Temperature effect on dielectric constant

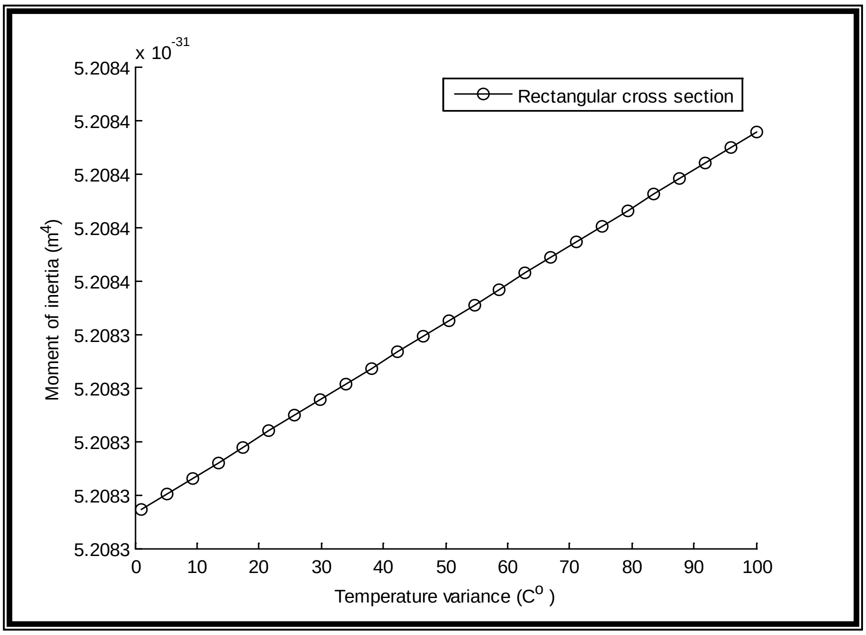
The relation between the dielectric constant , D_i, and temperature was shown in equation (14) and the result obtained is shown in figure(5) where an inverse relation can be seen.



Figure(5): The relation between dielectric constant and temperature for ZnO NW.

3-5 <u>Temperature effect on moment of inertia</u>

As we know the moment of inertia I depends on the shape of a beam's cross-section. Before determining the moment of inertia one must locate the centroid (neutral axis). Due to symmetry, the neutral axis runs through the centre of the cross-section. To evaluate I for a rectangle of height *l* and width b (figure (1)), the moment of inertia for a rectangular cross section is calculated using equation (5) and the result is shown in figure (6). A direct proportionality between the two quantities, minor increase in I can be seen.



Figure(6): The relation between moment of inertia and temperature variance (Δt) for a rectangular cross section ZnO NW with *l*,b = (600, 50) nm respectively.

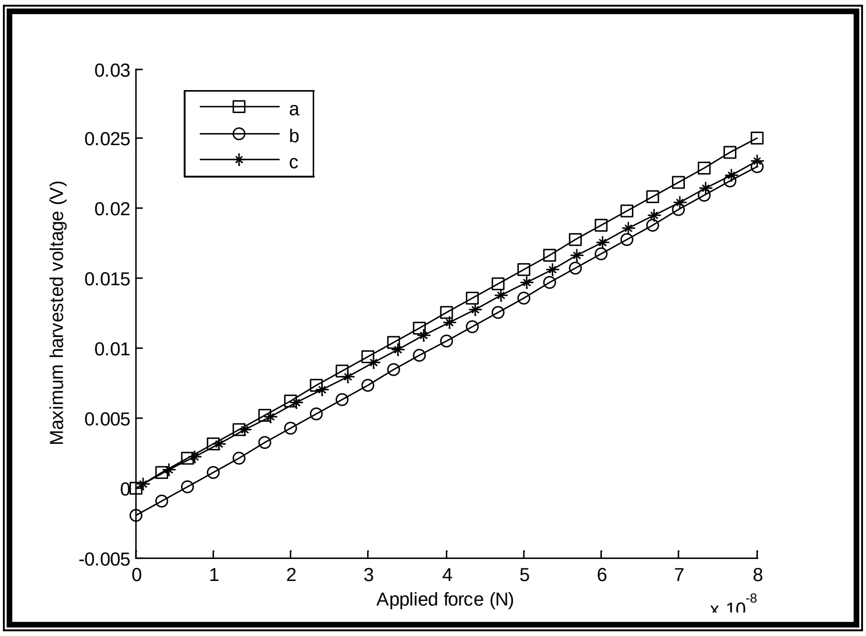
To figure-out the amount of harvested electrical energy for the cases:

a- No temperature effect i.e. by removing the temperature dependence given in equation (20).

b- With the effect of terms containing temperature effect given in equation (20).

c- Removing the temperature terms in equation (20) and substituting the definitions of young modulus (eq.12), stiffness constant(eq.13), ect.

We have solved equation (20) the results are shown in figure (7) where it can be seen that minor modification in the harvested electrical energy occurs.



Figure(7): Maximum harvested voltage against applied force for ZnO NW with rectangular cross section by solving eq.(20) for the situations: a-no effect of temperature, b- effect of temperature, c- effect of temperature on each parameter that depends on temperature.

4- Conclusion

The effect of temperature on various parameters of zing oxide (ZnO) NW such as young's modulus, dielectric, piezoelectric and elastic coefficients, poisson ratio and moment of inertia are studied. Obtained results prove that the temperature have sort of effect on these parameters. No major effects of increasing temperature on the overall harvested energy from ZnO NW have been noticed within the temperature range under which the ZnO nanowire can work.

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تأثير درجة الحرارة على خصائص مادة اوكسيد الزنك : حساب الطاقة الكهربائية المتولدة من اسلاك مصنوعة من مادة اوكسيد الزنك

رسول رمضان عتاب   جاسب عبد الحسين مشاري

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الخلاصة

في هذا العمل تم بيان تأثير درجة الحرارة على كل من معامل يونك، ثابت العزل، ثابت الكهربائية المتولدة من الضغط(الانضغاطية الكهربائية)، معامل المرونة، نسبة بوازون وكذلك عزم القصور الذاتي لمادة اوكسيد الزنك المرسبة على لوح ترسيب بأعتبارها مادة مولدة للشحنات الكهربائية عند تسليط قوة معينة(ضغط او انحناء). هذه المعاملات ذات اهمية في حساب الطاقة الكهربائية الناتجة من عملية انحناء اسلاك نانوية مصنوعة من مادة ZnO ذات ابعاد (طول وعرض) 50,600 نانومتر على التوالي عند تطبيق قوة خارجية بأستعمال مجهر نوع AFM (مجهر القوة الذرية) ضمن حدود المرونة.

لقد اثبتت النتائج ان هنالك تأثير عكسي لأختلاف درجة الحرارة مع كل من معامل يونك وثابت العزل للمادة المدروسة بينما اظهر اختلاف درجة الحرارة تأثير طردي (علاقة طردية) على بقية العوامل المدروسة.

ان تأثير اعتماد المتغيرات اعلاه على درجة الحرارة لم يؤثر كثيرا في الطاقة الكهربائية المستحصلة من الاسلاك النانوية المصنوع من مادة ZnO المرسبة على لوح ترسيب.