Flexoelectric effect on electric potential in piezoelectric graphene-based composite nanowire: Analytical and numerical modelling

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ABSTRACT

In this work, an analytical model was developed to study the distribution of electric potential in a graphene reinforced nanocomposite (GRNC) nanowire. The electromechanical responses such as electric potential and deflection of cylindrical GRNC cantilevered nanowire were investigated. Moreover, the conservative fully coupled finite element (FE) models were developed to validate the analytical predictions. Analytical solution shows that the piezoelectric potential in the GRNC nanowire depends on the transverse force, but it is not a function of the force acting along its axial direction. The electric potential in the tensile and compressive sections reveals that the flexoelectric effect on the electromechanical behavior of GRNC nanowire is noteworthy and cannot be ignored.

1. Introduction

The increase in demand of light-weight and high-strength materials in automobile and aerospace industries invites the researchers to use advanced technology for the development of new multifunctional engineering materials with superior thermo-mechanical and physical properties that are not met easily by conventional materials. Polymer nanocomposites are excellent structural materials that have desired and tailorable properties which can be used in a wide variety of applications. Recently, polymer matrix nanocomposite captivated the intense interest of the researchers due to its high specific stiffness and strength properties. Over the past two decades, to fulfil increasing demands of efficient, high-stiffness and mechanical strength of materials, several researchers experimentally incorporated the carbon-based nanostructures in conventional polymer matrices. In general, carbon nanofibers are identified as advanced nanomaterials with remarkable thermo-mechanical and electrical properties. A graphene layer is one of these materials, which is made of a two-dimensional monolayer of carbon atoms, arranged in hexagonal packing arrays. Several experimental and theoretical studies reported that the elastic modulus of a single graphene layer is about 1.0 TPa (Kundalwal et al., 2017, 2019; Selim et al., 2019; Shingare and Kundalwal, 2019). It is originated from its parent material graphite and is one of the most striking material of 21st century ever since it was discovered by Novoselov et al. (2004). This 2D monolayer amazed the researchers all over the world with its unique structure and remarkable scale-dependent physical properties. Recently, it was reported that it does not only possess remarkable thermomechanical properties but also show electromechanical coupling (Kundalwal et al., 2017). Using the density functional theory, Kundalwal et al. (2017) showed the presence of polarization in a non-piezoelectric and dielectric graphene layer via concept of flexoelectricity.

Piezoelectric, pyroelectric and ferroelectric materials are the family of dielectric materials which find a wider range of technologically significant applications such as sensors, actuators, capacitors, transducers, crack detection, artificial biological tissues etc. Piezoelectricity is the ability of certain materials that produce electric polarization when the strain is applied and vice-versa. Pyroelectricity is the ability of dielectric material to generate electric potential when temperature changes. Ferroelectricity is a characteristic of dielectric materials having perovskite structure that possess a spontaneous electric polarization which can be reversed by applying the external electric field. Curie temperature is an important parameter of such materials and their

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and the estimated value of flexoelectric coefficient can be considered as 

\[ \eta \approx 10^{-12} \text{ to } 10^{-13} \text{ C/m} \] (Jiang et al., 2013). Specifically, the pioneering work on the surface effect on nanostructure investigated by Shen and Hu (2010) using the theory of dielectrics accounting the influence of piezoelectric and flexoelectric effects with the consideration of surface parameters, which offers a mathematical framework to explore and compute the electromechanical response in nano-dielectrics. In a nanoscale ferroelectric material, by using the tip of an atomic force microscope (AFM), Lu et al. (2012) showed the induced stress gradient which can be utilized in NEMS.

Multifunctional graphene sheets find interesting high-value NEMS applications and owing to their extraordinary thermo-mechanical and electronic properties, graphene-based polymer nanocomposite materials have fascinated much attention (Zhu et al., 2014; Cui et al., 2016; Cui et al., 2016; Shen et al., 2017). Also, they can be used as chemical sensors because of their extraordinary sensitivity. These studies reported that the graphene-based nanocomposite can be a perfect replacement for conventional NEMS. Specifically, graphene-based polymer nanocomposite with good semiconductor properties (Yildirim and Ozturk, 2018), which makes it suitable to produce strain sensor having a high gauge factor. Hence, the investigation of the mechanical properties of graphene-reinforced polyimide (PI) nanocomposites is becoming extensively popular in the industry as well as academia. Recently, PI attracted a lot of attention due to its exceptional physico-thermo-mechanical properties in a wide temperature range. Its remarkable high-radiation resistance and better semiconductor properties can be utilized in various fields such as electrical and electronics applications as well as aviation industries. Further potential applications of PI with inorganic additives have fascinated extensive research investigations.

The most commonly used nanodevices are based on cylindrical nanowires that include piezoelectric field-effect transistors (FETs), piezoelectric resonators and nanoelectromechanical systems (Wang and Song, 2006; Wang, 2007). Piezoelectric NEMS have found the enormous potential for various applications such as energy harvesting and structural health monitoring (SHM) including electric switches, sensors, actuators, and nanogenerators (Deng et al., 2014). Particular structures such as nanobeams and nanoplates have certain restricted applications due to their geometrical configurations and the cylindrical nanowire is another key element to overcome the restrictions posed by beam and plates. The piezoelectric as well as flexoelectric effects in nanostructures play a significant role on their working mechanisms, especially nanowire-based nanogenerators. The working mechanism of nanowire-based nanogenerators largely depends on its deformation which generates electric polarization across its surface. For instance, Gao and Wang (2007) investigated the distribution of piezoelectric potential in cylindrical ZnO nanowire using the perturbation theory. They compared their analytical results with numerical FE simulations. Shao et al. (2010) proposed the simple continuum model for evaluating the distribution of electric potential generated in the cantilever nanorod bent by the uniform force applied at its tip. Momeni et al. (2010) developed the multi-physics analytical model to estimate the electric potential of ZnO nanocomposite. Recently, Shingare and Kundalwal (2020) studied the static response of graphene-based composite nanobeams subjected to end-point load with different boundary conditions considering the flexoelectric effect. They considered the upper and lower surfaces of graphene-based composites are electroded that illustrates the inverse effect of piezoelectricity and it can serve as a capacitor with two parallel plates where the hexagonal graphene sheets were reinforced into the polyimide matrix. The literature review indicates that the piezoelectric contribution in nanogenerators is studied by several researchers but to the best of current authors’ knowledge, there has been no single study on the incorporation of contribution of flexoelectric effect for investigating the distribution of electric potential in nanocomposite nanowire that may offer various opportunities for developing next-generation NEMS. This is indeed the inspiration behind the current work. The purpose of our investigation is to further widen the knowledge base of the presence of electric fields as well as strain gradients in GRNC nanowires. Therefore, the investigation of flexoelectric effect on the distribution of electric potential of GRNC nanowire is essential in nanogenerator design point of view. In this paper, we emphasise on the development of (i) a continuum model to determine the electric potential distribution of GRNC nanowire, and (ii) FE models to validate the electromechanical response of GRNC nanowire obtained by the analytical model.

2. Electromechanical response of GRNC nanowire

2.1. Effective properties of GRNC

The prediction of effective piezoelectric and elastic (piezoelectric) as well as dielectric properties of GRNC are required priori and therefore, its effective properties were determined first. We assumed graphene sheet as a piezoelectric continuum medium embedded in the PI matrix in 1–3 plane to form GRNC. Some existing experimental studies proved that the classical or continuum mechanics approach can be used to study the atomic-level graphene (Gong et al., 2010; Gupta and Batra, 2010; Shokrieh and Rafiee, 2016; Young et al., 2012; Cui et al., 2016; Papa-georgiou et al., 2017 and references therein). Therefore, we used mROM to determine the effective elastic properties of GRNC considering the geometrical factors of embedded graphene such as orientation, length and agglomeration. These factors are important as it is very difficult to obtain uniform dispersion and alignment of nanofillers in the matrix during the fabrication of nanocomposites. Krenchel orientation factor \( (\eta_{0}) \), critical length efficiency factor \( (\eta_{L}) \) and agglomeration factor \( (\eta_{A}) \) were taken into consideration as follows (Papa-georgiou et al., 2020):

\[ E_v = \eta_{0} \eta_{L} \eta_{A} E_v + \eta_{Vf} + E_m \nu_m \] (1)

The modified strength of materials (SOM) model in conjunction with Hill’s average concentration factor was used to determine the
piezoelectric and dielectric properties of GRNC. The detailed steps involved in the development of SOM are not presented here and readers are referred to Ref. (Shingare and Kundalwal, 2020) for more details.

2.2. Piezoelectricity and flexoelectricity effects

Fig. 2 demonstrates the configuration of GRNC nanowire as a nanogenerator. This mechanism is based on the deflection of piezoelectric nanowire through point load resulting in the distribution of electric potential in it. The principal material coordinate and problem coordinate systems are represented by x-y-z and 1-2-3, respectively, and these are exactly coincide with each other. The aim of the current study is to obtain a relationship between the applied transverse force \( f_x \) in x-direction and the distribution of electric dipoles in GRNC nanowire using both piezoelectric and flexoelectric effects. The free end of GRNC nanowire is subjected to the transverse force \( f_x \) that simulates the actual applied load or deflection.

According to the direct piezoelectric effect, the mechanical elastic strain induces the piezoelectric polarization in the piezoelectric material, which can be expressed as follows:

\[
P_i = e_{ijk} \varepsilon_{jk}
\]

where \( P_i \), \( \varepsilon_{jk} \) and \( e_{ijk} \) represent the polarization vector, second-order strain tensor and third-order linear piezoelectric tensor, respectively. According to Eq. (2a), the polarization induced due to the flexoelectric effect by small infinitesimal deformation follows the relation in terms of strain gradients as follows:

\[
P_i = e_{ijk} \varepsilon_{jk} + f_{ijkl} \frac{\partial \varepsilon_{jk}}{\partial x_l}
\]

in which \( f_{ijkl} \) is the fourth-order flexoelectric tensor. Using a relationship of the flexoelectric tensors, Shu et al. (2011) presented the symmetry of these coefficients in the crystalline medium as follows:

\[
f_{1111} = f_{2222} = f_{3333} = f_{11}
\]

\[
f_{1133} = f_{2233} = f_{1222} = f_{2121} = f_{1212} = f_{3311} = f_{1111}
\]

\[
f_{1212} = f_{1313} = f_{2132} = f_{2322} = f_{1223} = f_{3313} = f_{14}
\]

(3a)

For isotropic medium, the relationship between direct flexoelectric coefficients (Eq. (3a)) can be obtained as follows (Shu et al., 2011):

\[
f_{14} = \frac{1}{2} (f_{11} - f_{111})
\]

(3b)

After some manipulation, for the simplification purpose, above flexoelectric coefficients can be written as:

\[
f_{14,18} = \begin{pmatrix}
    f_{11} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & f_{14} & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

(4)
Furthermore, in case of isotropic materials, there is a relationship between the flexoelectric coefficients $f_{11}, f_{111}$ and $f_{14}$, and these independent coefficients can be reduced to two. The polarization charges in nanowire generated due to the piezoelectric and flexoelectric effects are bound charges instead of free charges. So, in absence of free charges, the Gauss’s law yields to:

$$\nabla \cdot \mathbf{D} = \rho_0 = 0$$ (5)

Here, for the cylindrical nanowire, the surface charge density ($\rho_0$) is 0, and $\mathbf{D}$ denotes a component of the electric displacement that can be obtained as follows:

$$\mathbf{D} = -\chi \nabla \phi + \mathbf{P}$$ (6)

where $\phi$ and $\chi$ represent the corresponding electric potential and relative permittivity of GRNC.

### 2.3. Continuum model of GRNC nanowire

We considered GRNC as a continuum medium and accordingly, the continuum mechanics based analytical model was developed. We consider the GRNC nanowire having a cylindrical shape with constant cross-sectional area of length $L$ and diameter $2a$. The flexoelectric coefficients of GRNC can be obtained from Eqs. (3b) and (4). The relationship between the stresses and strains in nanowire can be expressed as follows:

$$
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{33} \\
\gamma_{23} \\
\gamma_{31} \\
\gamma_{12}
\end{pmatrix} = \frac{1}{E}
\begin{pmatrix}
1 - \mu & -\mu & 0 & 0 & 0 \\
-\mu & 1 - \mu & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2(1 + \mu) \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2(1 + \mu)
\end{pmatrix}
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\tau_{23} \\
\tau_{31} \\
\tau_{12}
\end{pmatrix}
$$ (7)

We assumed that the free end of GRNC nanowire is purely subjected to the transverse force ($f_z$) and no torque is induced in it. Hence, according to Saint-Venant’s pure bending theory, the stress generated in nanowire can be expressed as follows (Green and Zerna, 2012):

$$
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\tau_{23} \\
\tau_{31} \\
\tau_{12}
\end{pmatrix} = \begin{pmatrix}
0 \\
-f_z \frac{1}{8} x(L-z) \\
0 \\
-f_z(3 + 2\mu) \\
0 \\
0
\end{pmatrix}
$$ (8)

where $I = (\pi/4) a^4$ is the moment of inertia of nanowire. By making use of Eqs. (7) and (8), the strain field in the nanowire can be obtained as:

$$
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{33} \\
\gamma_{23} \\
\gamma_{31} \\
\gamma_{12}
\end{pmatrix} = \frac{f_z}{E}
\begin{pmatrix}
\mu(L-z)x \\
\mu(L-z)x^2 - x(L-z) \\
\mu(L-z)x^2 - x(L-z) \\
\frac{1}{4}(1 + 2\mu) \\
0 \\
0
\end{pmatrix}
$$ (9)

in which non-zero strain gradient components are

$$\epsilon_{112} = \frac{f_z}{E}, \epsilon_{113} = \frac{f_z}{E}, \epsilon_{223} = \frac{f_z}{E},$$

$$\epsilon_{33,2} = \frac{f_z}{E}(L-z), \epsilon_{33,3} = \frac{f_z}{E}(L-z).$$

Hence, the material can be known as piezoelectric and flexoelectric when it provides polarization (electric response) due to the non-zero strain and strain gradient, respectively, and it can be seen in Eqs. (2a) and (2b).

By solving the simultaneous Eqs. (2b), (3), (4), (9) and (10), we have

$$P = \frac{f_z}{E}
\begin{pmatrix}
-\frac{1}{\chi} e_{15}xy \\
\frac{3 + 2\mu}{4} e_{15} \left( a^2 - y^2 - \frac{1 - 2\mu}{3 + 2\mu} x^2 \right) + F(L-z) \\
2\mu e_{21} - c_{31} x(L-z) + x[f_{11} - 2f_{11} + 1(1 + \mu) - 2f_{14}]\mu
\end{pmatrix}$$ (11)

where $F = \mu f_{11} + f_{14} L - f_{14}$.

The polarization effects in the nanowire due to the piezoelectricity are bound charges instead of free charges. Hence, the electric charge density in the GRNC nanowire can be introduced as:

$$\rho_0 = -\nabla \cdot P = \frac{f_z}{E}
\begin{pmatrix}
\frac{[2(1 + \mu)e_{21} + 2pe_{31} - e_{33}]x}{L-z} \\
\frac{[2(1 + \mu)e_{21} + 2pe_{31} - e_{33}]x}{L-z} \\
\frac{[2(1 + \mu)e_{21} + 2pe_{31} - e_{33}]x}{L-z}
\end{pmatrix}$$ (12)

where $A = \frac{f_z}{E} \frac{[2(1 + \mu)e_{21} + 2pe_{31} - e_{33}]x}{L-z}$.

By combining Poisson’s Eqs. (5) and (6), the relationship between the electric charge density ($\rho_0$) and electric potential ($\phi$) can be obtained as follows:

$$\nabla^2 \phi = -\frac{\rho_0}{\epsilon}$$ (13)

Subsequently, Poisson’s Eqs. (5) and (6) formulated in the form of cylindrical coordinates as follows:

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} = \frac{\rho_0}{\epsilon} - \frac{\partial f_z}{\chi} \sin \theta$$ (14)

Initially, Eq. (14) is solved by a combination of the general solution ($\phi^g$) of the homogeneous differential equation and particular solution ($\phi^p$), which is independent of $z$ coordinate. To solve the general solution, we can ignore the terms on right-hand side of Eq. (14) considering $\phi^g = R(r, \theta)Z(z)$. Thus, Eq. (14) can be re-written as

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial R}{\partial r} \right) + \frac{1}{r} \frac{\partial^2 R}{\partial \theta^2} + \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = 0$$ (15)

The first two terms are functions of $r$ and $\theta$, while the third term is a function of $z$. Hence, to solve Eq. (15), functions $R$ and $Z$ must fulfill the condition expressed by the below relations:

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial R}{\partial r} \right) + \frac{1}{r} \frac{\partial^2 R}{\partial \theta^2} = q^2$$ (16a)

$$\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} = -q^2$$ (16b)

where $q$ is a constant. To obtain an exact solution, the constant $q$ must be equal to 0. Hence, $Z(z) = A_1 z + A_2$ (17)

in which $A_1$ and $A_2$ are unknown coefficients. By using the procedure of series expansion of $R$ with suitable functions, Eq. (16a) can be solved and the function $R(r, \theta)$ can be expressed as:
\[ R(r, \theta) = R_0(r) + \sum_{n=1}^\infty \left[ R_{a_1}(r) \cos(n\theta) + R_{a_2}(r) \sin(n\theta) \right] \]  

(18)

Consequently, by determining \( R_0(r) \), \( R_{a_1}(r) \) and \( R_{a_2}(r) \), the expression of \( R(r, \theta) \) can be obtained. Substituting Eq. (18) into Eq. (16a), the corresponding equations can be obtained as:

\[ \frac{\partial}{\partial r} \left( \frac{\partial R}{\partial r} \right) = 0 \]  

(19a)

\[ \frac{\partial}{\partial r} \left( \frac{\partial R_{a_1}}{\partial r} \right) - \frac{n^2 R_{a_1}}{r^2} = 0, \quad n = 1, 2, 3... \]  

(19b)

\[ \frac{\partial}{\partial r} \left( \frac{\partial R_{a_2}}{\partial r} \right) - \frac{n^2 R_{a_2}}{r^2} = 0, \quad n = 1, 2, 3... \]  

(19c)

Using Eq. (19a), we can obtain

\[ R_0(r) = B_1 \ln(r) + B_2 \]  

(20)

In Eq. (19) (b) and (c), the terms \( R_{a_1}(r) \) and \( R_{a_2}(r) \) can be obtained as follows:

\[ R_{a_1}(r) = g_{a_1} r^n + h_{a_1} r^{-n}, \quad n = 1, 2, 3... \]  

(21a)

\[ R_{a_2}(r) = g_{a_2} r^n + h_{a_2} r^{-n}, \quad n = 1, 2, 3... \]  

(21b)

where \( B_1, B_2, g_{a_1}, h_{a_1}, g_{a_2} \) and \( h_{a_2} \) are unknown coefficients. Subsequently, the solution of Eq. (18) can be re-expressed as:

\[ R(r, \theta) = R_0(r) + \sum_{n=1}^\infty R_{a_1}(r)J + \sum_{n=1}^\infty R_{a_2}(r)K \]

\[ = B_1 \ln(r) + B_2 + \sum_{n=1}^\infty (g_{a_1} r^n + h_{a_1} r^{-n})J + \sum_{n=1}^\infty (g_{a_2} r^n + h_{a_2} r^{-n})K \]  

with \( J = \cos(n\theta) \) and \( K = \sin(n\theta) \). Hence, the general solution \( \varnothing^\# \) of Eq. (14) can be expressed as:

\[ \varnothing^\# = R(r, \theta)Z(z) \]

\[ \varnothing^\# = \left[ B_1 \ln(r) + B_2 + \sum_{n=1}^\infty (g_{a_1} r^n + h_{a_1} r^{-n})J \right] \]

\[ + \sum_{n=1}^\infty (g_{a_2} r^n + h_{a_2} r^{-n})K \left( \frac{A_1 r^3 + A_2}{r^3} \right) \]  

(23)

The solution of Eq. (24) is equal to the particular solution \( \varnothing^\# \) of Eq. (14) and it can be formulated as:

\[ \frac{\partial}{\partial r} \left( \frac{\partial \varnothing^\#}{\partial r} \right) + \frac{1}{r} \frac{\partial \varnothing^\#}{\partial r} = - \frac{A r}{r^3} \sin \theta \]  

(24a)

By using the approach of series expansion of \( \varnothing^\# \) with suitable functions, Eq. (24) can also be determined as follows:

\[ \varnothing = \left[ \left( \frac{B_1}{r^2} + \sum_{n=1}^\infty \frac{(g_{a_1} r^n + h_{a_1} r^{-n})J}{r^2} + C_1 \frac{A_{r^3}}{r^3} \sin \theta + \sum_{n=1}^\infty (C_{a_1} r^n)J + \sum_{n=1}^\infty (C_{a_2} r^n)K, \quad r \leq a \right) \right] e_x + C_2 \]

\[ \left[ \sum_{n=1}^\infty (h_{a_1} r^{-n})J + \sum_{n=1}^\infty (h_{a_2} r^{-n})K \right] (\frac{C_3}{r}) \sin \theta + \sum_{n=1}^\infty (C_{a_1} r^n)J + \sum_{n=2}^\infty (C_{a_2} r^n)K, \quad r > a \]  

(29b)

One can obtain a piecewise function divided by \( r = a \) using the boundary conditions \( \varnothing(r = 0) \neq 0 \) and \( \varnothing(r = \infty) = 0 \) when \( r > a \), \( A = 0 \); as follows:

\[ \varnothing^\#(r, \theta) = \varnothing_0(r) + \sum_{n=1}^\infty \varnothing_{a_1}(r)J + \varnothing_{a_2}(r)K \]  

(25)

Then, by calculating \( \varnothing_0(r), \varnothing_{a_1}(r) \) and \( \varnothing_{a_2}(r) \), the expression of \( \varnothing^\# \) can be derived. One can obtain the series of following Eq. (26a – 26d) by substituting Eq. (25) into Eq. (24); as follows:

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \varnothing_{a_1}}{\partial r} \right) = \]  

(26a)

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \varnothing_{a_2}}{\partial r} \right) + \frac{A_1}{r^3} \varnothing_{a_2} = - \frac{A r}{r^3} \sin \theta \]  

(26b)

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \varnothing_{a_2}}{\partial r} \right) - \frac{n^2 \varnothing_{a_2}}{r^2} = 0, \quad n = 1, 2, 3... \]  

(26c)

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \varnothing_{a_2}}{\partial r} \right) - \frac{n^2 \varnothing_{a_2}}{r^2} = 0, \quad n = 1, 2, 3... \]  

(26d)

The solutions of Eq. (26a – 26d) can obtained using the following relations:

\[ \varnothing_0(r) = C_1 \ln(r) + C_2 \]  

(27a)

\[ \varnothing_{a_2}(r) = C_3 r^4 - \frac{A r^3}{8r} \]  

(27b)

\[ \varnothing_{a_1}(r) = C_4 r^n + d_4 r^{-n}, \quad n = 1, 2, 3... \]  

(27c)

\[ \varnothing_{a_2}(r) = C_5 r^n + d_5 r^{-n}, \quad n = 2, 3, 4... \]  

(27d)

In which \( C_1, C_2, C_3, C_4, C_{a_1}, C_{a_2} \) and \( d_{a_2} \) are unknown coefficients. Hence, particular solution \( \varnothing^\# \) can be formulated as follows:

\[ \varnothing = \varnothing_0 + \varnothing^\# \]

\[ = \left[ B_1 \ln(r) + B_2 + \sum_{n=1}^\infty (g_{a_1} r^n + h_{a_1} r^{-n})J + \sum_{n=1}^\infty (g_{a_2} r^n + h_{a_2} r^{-n})K \right] \sum_{n=1}^\infty (C_{a_1} r^n)J + \sum_{n=1}^\infty (C_{a_2} r^n)K \left( \frac{A_1 r^3}{r^3} \right) \sin \theta + \sum_{n=2}^\infty (d_{a_1} r^n)J + \sum_{n=2}^\infty (d_{a_2} r^n)K \]  

(28)

Now, the solution of Eq. (14) can be formulated as:

\[ \varnothing = \varnothing_0 + \varnothing^\# \]

\[ = \left[ B_1 \ln(r) + B_2 + \sum_{n=1}^\infty (g_{a_1} r^n + h_{a_1} r^{-n})J + \sum_{n=1}^\infty (g_{a_2} r^n + h_{a_2} r^{-n})K \right] \sum_{n=1}^\infty (C_{a_1} r^n)J + \sum_{n=1}^\infty (C_{a_2} r^n)K \left( \frac{A_1 r^3}{r^3} \right) \sin \theta + \sum_{n=2}^\infty (d_{a_1} r^n)J + \sum_{n=2}^\infty (d_{a_2} r^n)K \]  

(29a)

Making the use of continuity conditions of the electric field ( \( \varnothing \) ) and charge at the surface (\( r = a \)) of GRNC nanowire and for obtaining all the unknown coefficients, the free space can be written as follows:
where m indicates the exterior normal unit vector (sinθ, cosθ, 0).

The following two equations can be obtained by substituting Eq. (29) into Eq. (30):

\[ \begin{align*}
B_3 + \sum_{n=1}^{\infty} (g_{n0} a^n) J + \sum_{n=1}^{\infty} (g_{n2} a^{n+1}) K & \cdot z + C_3 + \left( C_3 a - \frac{A_a^3}{8\sqrt{2}} \right) \sin \theta + \sum_{n=1}^{\infty} (d_{n1} a^n) J \\
+ \sum_{n=2}^{\infty} (c_{n2} a^n) K & = 0
\end{align*} \]

\[ \begin{align*}
E_3 + \sum_{n=1}^{\infty} (h_{n0} a^n) J + \sum_{n=2}^{\infty} (h_{n2} a^{n-1}) K & \cdot z + \left( \frac{C_3}{a} \right) \sin \theta + \sum_{n=1}^{\infty} (d_{n1} a^n) J \\
+ \sum_{n=2}^{\infty} (d_{n2} a^{n-1}) K & = 0
\end{align*} \]

(31a)

(31b)

Finally, the solution for the distribution of electric potential about the GRNC nanowire can be obtained as follows:

\[ \begin{align*}
\Omega |_{r=a} & = - \frac{f_3}{\text{EI} (\chi + X_0)} \int \left( \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{33}}{4} + (\mu f_{13}^2 - f_{14}) (L-z) \right) \sin \theta,
\end{align*} \]

\[ \begin{align*}
\Omega & = \begin{cases} 
\frac{f_3}{\text{EI} (\chi + X_0)} \left[ \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{31}}{4} + (\mu f_{13}^2 - f_{14}) (L-z) \right] \sin \theta, & r \leq a \\
- \frac{f_3}{\text{EI} (\chi + X_0)} \left[ \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{31}}{4} + (\mu f_{13}^2 - f_{14}) (L-z) \right] \sin \theta, & r > a 
\end{cases}
\]

(34)

and

\[ \begin{align*}
- \chi \left[ \sum_{n=1}^{\infty} (g_{n0} a^{n-1}) J + \sum_{n=2}^{\infty} (g_{n2} a^{n-1}) K \right] \cdot z + \left( C_3 - \frac{3A_a^3}{8\sqrt{2}} \right) \sin \theta \\
+ \sum_{n=2}^{\infty} (c_{n2} a^n) K & = 0
\end{align*} \]

(32a)

\[ \begin{align*}
- \chi \left[ \sum_{n=1}^{\infty} (h_{n0} a^{n-1}) J + \sum_{n=2}^{\infty} (h_{n2} a^{n-1}) K \right] \cdot z + \left( \frac{C_3}{a} \right) \sin \theta \\
+ \sum_{n=2}^{\infty} (d_{n2} a^{n-1}) K & = 0
\end{align*} \]

(32b)

The following system of equations can be obtained by comparing the coefficients of J and K appeared in Eqs. (31a) and (31b):

\[ \begin{align*}
g_{n0} a^n + c_{n0} a^n & = h_{n0} a^{n-1} + d_{n1} a^n - \left( \frac{A_a^3}{8\sqrt{2}} \right) \sin \theta \\
+ \sum_{n=2}^{\infty} (c_{n2} a^n) K & = 0
\end{align*} \]

(32a)

\[ \begin{align*}
- \chi \left[ \sum_{n=1}^{\infty} (g_{n0} a^{n-1}) J + \sum_{n=2}^{\infty} (g_{n2} a^{n-1}) K \right] \cdot z + \left( C_3 - \frac{3A_a^3}{8\sqrt{2}} \right) \sin \theta \\
+ \sum_{n=2}^{\infty} (c_{n2} a^n) K & = 0
\end{align*} \]

(32b)

\[ \begin{align*}
- \chi \left[ \sum_{n=1}^{\infty} (h_{n0} a^{n-1}) J + \sum_{n=2}^{\infty} (h_{n2} a^{n-1}) K \right] \cdot z + \left( \frac{C_3}{a} \right) \sin \theta \\
+ \sum_{n=2}^{\infty} (d_{n2} a^{n-1}) K & = 0
\end{align*} \]

(32c)

(32d)

where B_2, C_4, d_{n1}, d_{n2}, h_{n1}, h_{n2} and h_{n3} are unknown coefficients.

Then, by comparing the respective coefficients of z and constant terms in Eq. (32a – 32d), the expressions of coefficients in Eq. (29) can be determined as follows:

\[ \begin{align*}
g_{n0} & = c_{n0} = h_{n0} = d_{n0} = 0, n = 1, 2, 3, \ldots \\
g_{n2} & = c_{n2} = h_{n2} = d_{n2} = 0, n = 2, 3, 4, \ldots \\
B_2 & = g_{21} = h_{21} = d_{21} = C_2 = 0,
\end{align*} \]

\[ \begin{align*}
C_3 & = \frac{A_a^3 (3\chi + X_0)}{8\chi (\chi + X_0)} + \frac{F_3 L}{E_3 (\chi + X_0)} \\
C_4 & = \frac{A_a^4}{4\chi (\chi + X_0)} + \frac{F_3 L a^2}{E_3 (\chi + X_0)} \\
g_{12} & = - \frac{F_3}{E_3 (\chi + X_0)} h_{12} = - \frac{F_3 a^3}{E_3 (\chi + X_0)}
\end{align*} \]

(33)

Finally, the solution for the distribution of electric potential about the GRNC nanowire can be obtained as follows:

\[ \begin{align*}
\Omega & = \begin{cases} 
\frac{f_3}{\text{EI} (\chi + X_0)} \left[ \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{33}}{4} + (\mu f_{13}^2 - f_{14}) (L-z) \right] \sin \theta, & r \leq a \\
- \frac{f_3}{\text{EI} (\chi + X_0)} \left[ \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{33}}{4} + (\mu f_{13}^2 - f_{14}) (L-z) \right] \sin \theta, & r > a 
\end{cases}
\end{align*} \]

(34)

If the flexoelectric effect is not considered (f_{11} \rightarrow 0), then Eq. (34) reduces to

\[ \begin{align*}
\Omega & = \begin{cases} 
\frac{f_3}{\text{EI} (\chi + X_0)} \left[ \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{33}}{4} + (\mu f_{13}^2 - f_{14}) (L-z) \right] \sin \theta, & r \leq a \\
- \frac{f_3}{\text{EI} (\chi + X_0)} \left[ \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{33}}{4} + (\mu f_{13}^2 - f_{14}) (L-z) \right] \sin \theta, & r > a 
\end{cases}
\end{align*} \]

(35)

These estimates are in coherence with the results obtained by Shao et al. (2010). From above Eq. (35), the maximum potential is generated at the surface (r = a) of nanowire on the tension (θ = -90°) and compression (θ = +90°) sides, which can be written as:

\[ \varphi_{\text{max, com}} = \frac{f_3}{\pi E_3 (\chi + X_0)} \left[ \frac{2(1 + \mu) c_{13} + 2\mu c_{31} - e_{33}}{a} \right] \]

According to the theory of elasticity, as the GRNC nanowire is subjected to only transverse mechanical force (f_4) and then the maximum deflection can be obtained as follows (z = L):

\[ \delta_{\text{max}} = \frac{f_4 L^3}{8E_3 I_3} \]

(37)

Hence, from Eqs. (36) and (37), the maximum piezoelectric potential obtained in terms of maximum deflection is given by (f_{11} = f_{14} → 0):

\[ \varphi_{\text{max, com}} = \frac{3}{4(\chi + X_0)} \left[ \frac{(2(1 + \mu) c_{13} + 2\mu c_{31} - e_{33}) a^3}{L^3} \right] \delta_{\text{max}} \]

(38)
2.4. Finite element (FE) modelling

2.4.1. FE modelling of GRNC

Note that the mROM and SOM models used in Section 2.1 are based on some assumptions, and the FE analysis may be carried out to validate these assumptions. Therefore, the FE models were developed to validate the analytical predictions of effective properties of GRNC using ANSYS Parametric Design Language (APDL) 15.0 software. The 3D multi-field twenty noded coupled-field brick elements “solid 226” with linear interpolation were used to discretize or mesh the continuum of GRNC, where single node was having four DOF, with three displacement translations with respect to coordinate systems and one electric potential. The RVE of GRNC was discretized with quadrilateral elements, as shown in Fig. 1b. We used Eq. (39) to estimate the required averaged stresses (σij), strains (εij), electric field (Ei) and displacement (Di), and finally the effective elastic (C11, C12, C13, C33), piezoelectric (ε11, ε13, ε33) and dielectric (ε33) coefficients were evaluated using Eq. (40).

\[
\begin{align*}
\sigma_{ij} &= \frac{1}{V} \sum_{r=1}^{n} \sigma_{ij} V_r; \\
\varepsilon_{ij} &= \frac{1}{V} \sum_{r=1}^{n} \varepsilon_{ij} V_r; \\
D_i &= \frac{1}{V} \sum_{r=1}^{n} D_i V_r; \\
E_i &= \frac{1}{V} \sum_{r=1}^{n} E_i V_r
\end{align*}
\]

(39)

in which V and Vr represent the respective volumes of RVE and finite elements, and n denotes the number of finite elements. The detailed procedure for estimating the effective coefficients of GRNC by applying the proper loading and boundary conditions on the faces of its RVE is not described here for the sake of brevity and the same presented elsewhere (Kundalwal et al., 2019).

2.4.2. FE modelling of GRNC nanowire

In the FE analysis, the material and geometrical properties of GRNC nanowire are used same as that used in the analytical model. A commercially available software (ANSYS-APDL) was used for the FE analysis. Once again, the multi-field 20 noded “solid 226” brick elements with displacement and electric voltage DOF were used for FE modelling of GRNC nanowire. Fig. 3 illustrates the loading condition, distribution of piezoelectric potential and deformation of FE model of GRNC nanowire having 50 nm diameter which is subjected to only the mechanical transverse force. The meshing of GRNC nanowire was

![Fig. 3. GRNC nanowire: (a) loading condition with transverse force (f₄), (b) distribution of maximum and minimum electric potentials and (c) deformation.](image)

![Fig. 4. Variation of electric potential in the transverse cross-section of GRNC nanowire at z = 1/2 (=300 nm) with and without considering flexoelectricity.](image)
performed by using “Hexahedral-Quad” sweep type of element which results into 26923 and 5969 number of nodes and elements, respectively. The obtained FE results are discussed in Section 3.

2.4.3. Effects of surface and body charge densities

To predict the piezoelectric potential, the surface and body charge densities can be used as boundary conditions (Zhang et al., 2016) in the FE model. Contrast to the response of piezoelectricity, due to the surface charge, electric polarization is generated considering only the flexoelectric effect and body charge becomes very negligible. On both the end surfaces of nanowire, the surface charge density can be neglected because nanowire does not carry a substantial inherent electric field inside it because of its large aspect ratio.

3. Result and discussion

In this section, the results obtained from the continuum and numerical models are discussed. The effective properties of GRNC were estimated by considering 0.05 graphene volume fraction (5%) using the micromechanics models developed in Section 2.1. The values \( \eta_0, \eta_1 \) and \( \eta_s \) factors become unity in case of aligned and non-agglomerated graphene layers perfectly bonded with the surrounding matrix (Papageorgiou et al., 2020). Moreover, the FE simulations were carried out to validate the analytical predictions. The estimated values of effective properties of GRNC with 5% graphene volume fraction are summarized in Table 1 and we can observe that the comparison of analytical and FE predictions is in better agreement.

Our selection of use of volume fraction of graphene as 0.05 was based on the fact that several researchers fabricated nanocomposite samples with 5-90% volume fraction of graphene and its derivatives such as graphite or graphene oxide (GO) using unique nanofabrication techniques: dispersion method, layer-by-layer assembly and solution blending route (Gamboa et al., 2010; Gong et al., 2012; Young et al., 2012; Yang et al., 2013; Papageorgiou et al., 2017). A GRNC nanowire of diameter \( (2a) \) 50 nm and length 600 nm was considered. The thickness of single layer of graphene sheet was considered as 0.34 nm (i.e., distance between two atomic layer of multi-layered graphene). The CVD is one of the most common methods for the preparation of high-quality thin 2D films on the order of micrometer (Xu et al., 2014); therefore, a graphene layer having lateral dimensions on the order of nm can be fabricated using CVD. The assemblies of multi-layers of GO and polyethyleneimine were presented by tailoring the thickness of number of GO layers. In case of bilayer of GO and polyethyleneimine, the thickness of assembly near about \( \approx 5 \text{ nm} \) was achieved. In some other studies, the thickness of assembly was achieved in the range of 8-10 nm using 4 to 30 graphene platelets (Yang et al., 2013; Prolongo et al., 2014, 2018; Tzeng et al., 2015). Using these techniques, the fabrication of GRNC nanowire can be achieved on the order of nm.

Recently, an experimental investigation revealed that the flexoelectric coefficients for ceramics, polymers, elastomers and crystals are much more than the earlier approximations. Therefore, it is experimentally demonstrated that for certain ceramics, polymers, elastomers, and crystals, the flexoelectric coefficient was found to have the order of magnitude, \( e/a \approx 10^{-12} - 10^{-6} \text{C/m} \); in which ‘e’ and ‘a’ denote the electronic charge and lattice constant, respectively (Jiang et al., 2013; Kogan, 1964). By means of experimental methods, this has been established by Zubko et al. (2013) and we assumed the flexoelectric coefficient \( f_{11} \approx f_{14} \approx 10^{-9} \text{C/m} \). From Eq. (34), it can be noted that the electric potential is directly proportional to the transverse force on the nanowire. The free end of GRNC nanowire was subjected to the transverse force \( f_x = 80 \text{nN} \) for further analysis.

Fig. 4 illustrates the distribution of electric potential at different radii in the transverse cross-section of GRNC nanowire at \( z = 1/2 \) (≈300 nm) with and without considering flexoelectricity. It may be observed that there is substantial increase in the distribution of electric potential when the flexoelectric effect is considered \( (f_{11} = f_{14} = 1 \text{nC/m}) \). It can be observed from Fig. 4 that the electric potential in the tensile part of

![Fig. 5. The 3D representation of distribution and contours of electric potential in the transverse cross-section of GRNC nanowire at \( z = 1/2 \) (≈300 nm) (a) with and (b) without considering flexoelectricity.](image-url)
nanowire is positive while it is negative in the compressive part, and they are antisymmetric about the x-axis. The electric potential of GRNC nanowire is improved significantly when the flexoelectric effect is considered for the 50 nm diameter with the application of 80 nN force over that of a conventional nanowire (i.e., without flexoelectricity). From Figs. 3 and 4 it is clearly seen that the maximum and minimum values of electrical potential occur at the extreme surface along the length of nanowire have the opposite signs. All values are separated by a reference line of zero-valued electric potential in the mid of nanowire. According to our formulation, the first case \((r \leq a)\) of Eq. (34), the function of electric potential is directly proportional to the square of radius \((a^2)\) of nanowire but in the second case \((r > a)\) and \((r < -a)\) it is proportional to the fourth power of radius \((a^2)\) of nanowire. Therefore, the maximum value of electric potential is obtained when \(r = a\) in both the cases and it decreases when \(r < -a\) or \(r > a\) while it increases when \(r < a\). It is obviously seen from Eq. (38) that the maximum electric potential is directly proportional to the maximum deflection and inversely proportional to the aspect ratio of nanowire. The respective estimated values of electric potentials determined by using the analytical and FE models are 7.45 mV and 7.72 mV, and this comparison validates our analytical model. Fig. 5 demonstrates the 3D representation of distribution and contours of electric potential in the transverse cross-section of GRNC nanowire at \(z = 1/2\) (=300 nm) with and without considering flexoelectricity. It can be seen that the distribution of electric potential of GRNC nanowire considering the flexoelectric effect (Fig. 5a) shows the better enhancement compared to the distribution of electric potential without considering the flexoelectric effect (Fig. 5b). The colorbar in Fig. 5 represents clear increment in the value of electric potential. Contours under the mesh plot show the variation of electric potential along the length of nanowire plotted in x-y plane. Similar to Fig. 4 it is obviously seen that the maximum and minimum values of electrical potential occur at the extreme surfaces of nanowire. It is clearly observed from Figs. (3b) and (5b) that the colorbars show the good agreement between the analytical and FE predictions for the distribution of electric potential.

Fig. 7 depicts the variation of electric potential in the transverse cross-section of GRNC nanowire at \(z = 1/2\) (=300 nm) with and without considering flexoelectricity. It can be seen that the distribution of electric potential is improved significantly when the flexoelectric effect is considered for the 50 nm diameter with the application of 80 nN force over that of a conventional nanowire (i.e., without flexoelectricity). From Figs. 3 and 4 it is clearly seen that the maximum and minimum values of electrical potential occur at the extreme surface along the length of nanowire have the opposite signs. All values are separated by a reference line of zero-valued electric potential in the mid of nanowire. According to our formulation, the first case \((r \leq a)\) of Eq. (34), the function of electric potential is directly proportional to the square of radius \((a^2)\) of nanowire but in the second case \((r > a)\) and \((r < -a)\) it is proportional to the fourth power of radius \((a^2)\) of nanowire. Therefore, the maximum value of electric potential is obtained when \(r = a\) in both the cases and it decreases when \(r < -a\) or \(r > a\) while it increases when \(r < a\). It is obviously seen from Eq. (38) that the maximum electric potential is directly proportional to the maximum deflection and inversely proportional to the aspect ratio of nanowire. The respective estimated values of electric potentials determined by using the analytical and FE models are 7.45 mV and 7.72 mV, and this comparison validates our analytical model. Fig. 5 demonstrates the 3D representation of distribution and contours of electric potential in the transverse cross-section of GRNC nanowire at \(z = 1/2\) (=300 nm) with and without considering flexoelectricity. It can be seen that the distribution of electric potential of GRNC nanowire considering the flexoelectric effect (Fig. 5a) shows the better enhancement compared to the distribution of electric potential without considering the flexoelectric effect (Fig. 5b). The colorbar in Fig. 5 represents clear increment in the value of electric potential. Contours under the mesh plot show the variation of electric potential along the length of nanowire plotted in x-y plane. Similar to Fig. 4 it is obviously seen that the maximum and minimum values of electrical potential occur at the extreme surfaces of nanowire. It is clearly observed from Figs. (3b) and (5b) that the colorbars show the good agreement between the analytical and FE predictions for the distribution of electric potential.

Fig. 6 shows the variation of electric potential at different transverse cross-sections of GRNC nanowire along its length \((z)\) considering the flexoelectricity. This figure illustrates the distribution of electric dipoles inside the GRNC nanowire with cantilever boundary condition and body charge. As expected, it can be observed that the electric potential decreases as the length \((z)\) of nanowire increases and at \(z = l\), it reaches to a minimum value. This is attributed to the fact that the stresses (tensile and compressive) are maximum at the fixed end of beam \((z = 0)\) and their values start decreasing as the point of interest along its length moves towards the free end \((z = l)\). This results in the larger strain gradients at the fixed end of beam which eventually shows the higher electric potential. The distribution of electric potential reveals the behavior like a “parallel plate capacitor” (Fig. 3). Because of the relatively small diameter compared to the length of nanowire, the charges on both ends of nanowire shows an insignificant effect on the electric field.

Next, we considered different values of flexoelectric coefficients. For the first set, we considered the same magnitude of flexoelectric coefficients: \(f_{11} = f_{14} = 1\text{nC/m} ; f_{11} = f_{14} = -1\text{nC/m} ; f_{11} = f_{14} = 0\text{nC/m}\). For the other set, we considered the different values: \(f_{11} = 0.75\text{nC/m} \) and \(f_{14} = 1.25\text{nC/m} ; f_{11} = 0.5\text{nC/m} \) and \(f_{14} = 2.0\text{nC/m} \); and \(f_{11} = 2.0\text{nC/m} \) and \(f_{14} = 0.5\text{nC/m} \). Fig. 7 depicts the variation of electric potential in the transverse cross-section of GRNC nanowire at \(z = 1/2\) (=300 nm) considering different values of flexoelectric constants. It can be noticed that the incorporation flexoelectric effect significantly influences the distribution of electric potential of

Fig. 7. Variation of electric potential in the transverse cross-section of GRNC nanowire at \(z = 1/2\) (=300 nm) considering different values of flexoelectric constants.

Fig. 8. Variation of electric potential against the diameter of GRNC nanowire in its transverse cross-section at \(z = 1/2\) (=300 nm) considering flexoelectricity.

Fig. 9. Variation of electric voltage \((\langle V_f - V_c \rangle)/\langle V_c \rangle)\) against the radius of GRNC nanowire in its transverse cross-section at \(z = 1/2\) (=300 nm).
GRNC nanowire compared to that of the conventional nanowire \( f_{11} = f_{14} = 0 \text{nC/m} \). This is attributed to the fact that the term \( \frac{d_{11} - d_{14}}{d_{11} + d_{14}} \) in Eq. (34) influences the distribution of electric potential of GRNC nanowire in which \( f_{11} \) and \( f_{14} \) are the longitudinal and shear flexoelectric coefficients, respectively. It can be observed that the shear flexoelectric coefficient largely influences the response compared to that of the longitudinal flexoelectric coefficient but usually the latter is larger than that of the former in magnitude.

Fig. 8 illustrates the variation of electric potential against the diameter of GRNC nanowire in its transverse cross-section at \( z = 1/2 \) (≈300 nm) considering flexoelectricity. Five discrete values of diameters of GRNC nanowires were considered: 30 nm, 40 nm, 50 nm, 60 nm and 70 nm. As expected it can be observed that on decreasing the diameter the voltage increases because the flexoelectric effect is a size-dependent phenomenon. Hence, it is obvious that the flexoelectric effect cannot be neglected for studying the electromechanical behavior of thin structures. The relative difference of electric voltage \( \frac{(V_f - V_0)}{V_0} \) is the ratio of difference of electric voltages of GRNC nanowire with and without considering the flexoelectric effect \( \frac{(V_f - V_0)}{V_0} \) and without considering the flexoelectric effect \( V_0 \). Fig. 9 demonstrates the variation of electric voltage \( \frac{(V_f - V)}{V_0} \) against the radius of GRNC nanowire in its transverse cross-section at \( z = 1/2 \) (≈300 nm). It can be noticed from Figs. 8 and 9 that the flexoelectric effect is more dominant for smaller diameter of nanowires indicating that the flexoelectric effect becomes negligible when the diameter of nanowire increases. Thus, the current results obviously reveal that the flexoelectric effect should be considered in case of bending or stretching of smaller diameter nanowires.

The variation of deflection of end point of GRNC nanowire (at \( z = 1 \) (≈600 nm)) against the transverse force imposed on its top surface is shown in Fig. 10. It is noticed that the value of deflection \( \delta_{\text{max}} \) increases linearly with the applied transverse force. According to the simple theory of elasticity, when the piezoelectric GRNC nanowire subjected to the transverse mechanical load considering only body charge, then the solution behaves as per the elastic homogeneous solution for deflection (see Eq. (37)). From Eq. (37), it can be noted that the maximum deflection of nanowire is directly proportional to the applied transverse force and cube of length of nanowire. The respective estimated values of maximum deflection of nanowire determined using the analytical and FE models are 352.6 nm and 352.00 nm, and this comparison validates our analytical model. Results illustrated in Figs. 4–10 clearly reveal that the electric potential distribution of GRNC nanowire is significantly influenced by the incorporation of flexoelectric effect and one can tailor the electromechanical response of nanowires and thin nanostructures by varying their geometrical parameters such as radius, length and volume fraction of nanoreinforcements. Obtained results produce a fundamental basis and suggest new parameters for investigation of the electromechanical response of nanowires which find interesting NEMS applications such as field effect transistors (FETs), nanopiezotronics, piezoelectric nanogenerators, gated diode, resonators, etc.

4. Conclusions

An analytical model was developed for studying the distribution of electric potential in GRNC nanowire accounting the flexoelectric effect. The electromechanical responses such as electric potential and deflection of GRNC nanowire were investigated. The FE models were also developed to validate the analytical predictions. The following is a summary of the current results:

- The piezoelectric potential in the GRNC nanowire depends on the transverse force but it is not a function of force acting along its axial direction.
- Electric potential distribution in the tensile and compressive sections of nanowire is antisymmetric along its cross-section, which makes it a “parallel plate capacitor” for the application of nanopiezotronics devices.
- The shear flexoelectric coefficient largely influences the response of GRNC nanowire compared to that of the longitudinal flexoelectric coefficient.
- The flexoelectric effect is more dominant for smaller diameter of GRNC nanowires and it cannot be ignored in case of bending or stretching of smaller diameter nanowires as well as composite nanostructures.

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References


