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RVE Analysis of Light Weight Carbon Nanotubes Embedded Piezoelectric Fibre Composites

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Abstract The hybrid piezoelectric composite comprised of carbon nanotubes and piezoelectric fibres as reinforcements embedded in a polyvinylidenedifluoride (PVDF) matrix is investigated. Effective elastic and piezoelectric properties of hybrid piezoelectric composite have been determined by the representative volume element (RVE) based on the finite element method. The results show that effective elastic coefficients and dielectric piezoelectric coefficient increases with increasing the volume fraction whereas piezoelectric coefficients e13, e23 and e33 are equal due to transversaly isotropy and decreases with increasing volume fraction. However, piezoelectric coefficients e42 and e51increases with increasing of volume fraction.

Keywords Carbon nanotubes, Polyvinylidene difluoride, Elastic properties, Homogenization method

1. Introduction

Piezoelectric composites, often, called piezocomposites, have been used as distributed actuators and sensors. Piezocomposites (PZCs), usually comprised of an epoxy reinforced with a monolithic piezoelectric material (PZT), provide a wide range of effective material properties not offered by existing PZTs, are anisotropic, and characterized by good conformability and strength. Even through their properties make them interesting, they are often limited, first by their weight, that can be a clear disadvantage for shape control and, as a consequence, by their high specific acoustic impedance, which reduces their acoustic matching with the external fluid domain. Bulk piezoelectric materials have several drawbacks, and hence composite materials are often a better technological solution in the case of many applications such as in ultrasonic transducers, medical imaging, sensors, actuators and damping. In recent years, composite piezoelectric materials have been developed by combining piezoceramics with passive non-piezoelectric polymers. Superior properties have been achieved with these composites by taking advantage of the most beneficial properties of each constituent and a great variety of structures have been made [1-3].

Recently, polymeric nanocomposites filled with such nanoparticles as carbon nanotubes (CNTs), nanoclays, and have nanofibres have attracted a large amount of attention to achieve more enhanced mechanical, thermal, and electrical properties than conventional composites [4-6]. Especially, CNT has outstanding elastic modulus and tensile strength over the other nanoparticles. Many experimental investigations on mechanical properties of the CNT filled nanocomposites have been carried out but more studies are needed to realize the potential of CNTs as reinforcement [7-9]. In order to obtain a composite structure with tunable properties ranging from stiffer structure to better damper, the quality of adhesion between nanotube and matrix needs to be manipulated. In this regard, the restriction effect of nanotube on the surrounding polymeric matrix plays an important role. Salehi et al [10] proposed a continuous radiation model for a nano-epoxy system with an interphase layer around a nanomaterial. They showed that as the distance of polymeric segment and nanomaterial increases, the restriction effect of nanomaterial on the segment decreases gradually. Therefore, the farther segments are to the nanomaterial, the less immobilization of segments is formed. Also, interfacial slip is activated at the nanotube-polymer interfaces by raising the temperature. Therefore, at higher temperature the molecule density in the interphase zone decreases due to thermal expansion effects. To make this concept more powerful in term of response time polyvinylidene fluoride (PVDF) matrix is more useful than the polymer matrix. On the other hand, PVDF is very flexible, exhibits good stability over time and does not depolarize when subjected to very high alternating electric field. In order to enhance the necessary properties of PVDF with other organic or inorganic blends was recently investigated. Moreover, PVDF elements appear

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to have certain advantages in comparison with their piezoceramic counterparts. At present, PVDF polymer is produced in the form of thin film of thickness ranging from 102 x 10^{-4} to 762 x 10^{-3} mm. Utilizing ferroelectric ceramic particles or metal particles as a dispersed phase in piezoelectric polymer matrix has its own merits but suffers some drawbacks such as no uniform poling or suffering fatigue or early failure under cycling as well as dispersion of large particles, originated from the immiscibility. However, PVDF-multi-walled carbon nanotube (MWCNT) composites showed that the elevation of piezoelectric β form crystal was increased with MWCNT amount when subjected to poling. Besides the stretching and poling in the PVDF films, addition of MWCNT enhanced the β phase content by acting as nucleating agent and then its piezoelectric property, too [11-14].

In the present study, the effective piezoelectric properties of the CNT / PVDF nanocomposite embedded with piezoelectric composite is examined by using the representative volume element (RVE) homogenization method.

2. Piezoelectric Constitutive Equations

The behavior of the piezoelectric medium is described by the following piezoelectric constitutive equations, which correlate stresses (T), strains (S), electric field (E), and electrical displacement (D) as given below [1];

$$\begin{bmatrix} T \\ D \end{bmatrix} = \begin{bmatrix} C & -e^T \\ e & k \end{bmatrix} \begin{bmatrix} S \\ E \end{bmatrix} \tag{1}$$

where C is the elasticity matrix,$k$is the permittivity matrix, and e is the piezoelectric strain coupling matrix.

For a transversely isotropic piezoelectric solid, the stiffness matrix, the piezoelectric matrix and the dielectric matrix simplify so there remain in all 11 independent coefficients. In the case of aligned fibers made of a transversely isotropic piezoelectric solid (PZT), embedded in an isotropic polymer matrix, the resulting composite is a transversely isotropic piezoelectric material (crystal class 6 mm) for a hexagonal array and tetragonal (crystal class 4 mm) for a square array. Consequently, the constitutive equation (1) for the composite can be written as [1];

$$\begin{bmatrix} \overline{T}_{11} \\ \overline{T}_{22} \\ \overline{T}_{33} \\ \overline{T}_{23} \\ \overline{T}_{31} \\ \overline{T}_{12} \\ \overline{D}_{1} \\ \overline{D}_{2} \\ \overline{D}_{3} \end{bmatrix} = \left[\begin{array}{cccccc|ccc} C_{11}^{eff} & & & & & & 0 & 0 & -e_{13}^{eff} \\ C_{21}^{eff} & C_{22}^{eff} & & & symm. & & 0 & 0 & -e_{23}^{eff} \\ C_{31}^{eff} & C_{32}^{eff} & C_{33}^{eff} & & & & 0 & 0 & -e_{33}^{eff} \\ 0 & 0 & 0 & C_{44}^{eff} & & & 0 & -e_{42}^{eff} & 0 \\ 0 & 0 & 0 & 0 & C_{55}^{eff} & & -e_{51}^{eff} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66}^{eff} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & e_{15}^{eff} & 0 & k_{11}^{eff} & & symm. \\ 0 & 0 & 0 & e_{24}^{eff} & 0 & 0 & 0 & k_{22}^{eff} & \\ e_{31}^{eff} & e_{32}^{eff} & e_{33}^{eff} & 0 & 0 & 0 & 0 & 0 & k_{33}^{eff} \end{array}\right] \cdot \begin{bmatrix} \overline{S}_{11} \\ \overline{S}_{22} \\ \overline{S}_{33} \\ \overline{S}_{23} \\ \overline{S}_{31} \\ \overline{S}_{12} \\ \overline{E}_{1} \\ \overline{E}_{2} \\ \overline{E}_{3} \end{bmatrix} \tag{2}$$

In both cases except that $C_{11}^{eff} - C_{12}^{eff} = 2\,C_{66}^{eff}$ for 6mm symmetry.

3. Results and Discussion

Fig.1. schematically shows the procedure of homogenization technique used in this study.

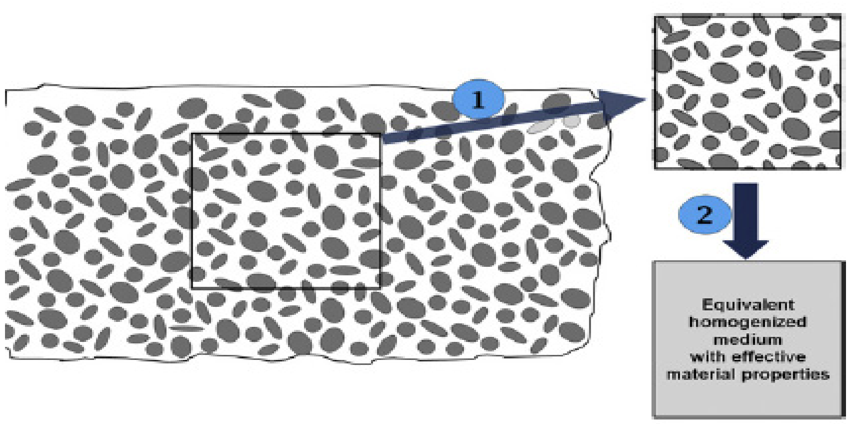


Figure 1. Selection of modelling volume 1 and homogenization medium 2

To implement the numerical homogenization, Finite Element Method which looks promising in addition to being readily available, is utilized here. The RVE regions consist of air, CNTs, and matrix. The RVE is constructed based on the following assumptions; (i) the CNTs are homogeneously dispersed in the nanocomposites with the square packing, (ii) they are perfectly bonded with the matrix and have uniform dimensions such as their length, inner, and outer diameters, (iii) there is no direct interaction between the adjacent CNTs, (iv) the CNT nanocomposites contain the periodic unit cell which includes a single CNTs are loaded in the nanocomposites so that the above assumptions should be valid. For the numerical simulations of the proposed piezo nanocomposites, the physical as well the geometrical properties of the constituents are required as inputs. Material properties of CNT, taken from Ref. [5], and of the PDVF are given below Table 1.

The overall behavior of the composite depends mainly on the volume fraction of the nanotubes. The effective properties increases with increase of volume fraction, which includes volume of nanotubes, should be placed in the same volume. The same effect can be achieved by reducing the size of the unit cell [2]. But finally it is also possible to keep the size of the unit cell constant and to enlarge the included nanotube by keeping the geometrical relations length/radius (l/r = 4/3) and thickness/radius (t/r=0.2). In this sense, unit cell models were created for volume fractions between 0.025 (2.5 %) and 0.15 (15 %) in steps of 2.5 %.

Fig. 2 shows the model with the lowest and highest volume fraction. The nanotubes are aligned in x3 direction because of alignment of the nanotube in x3 direction. The overall behavior is transversely isotropic [3]. Then the equality between the following coefficients must be exit: C11= C22, C31= C32, C44= C55, e31= e32, e15= e24, k11= k22.

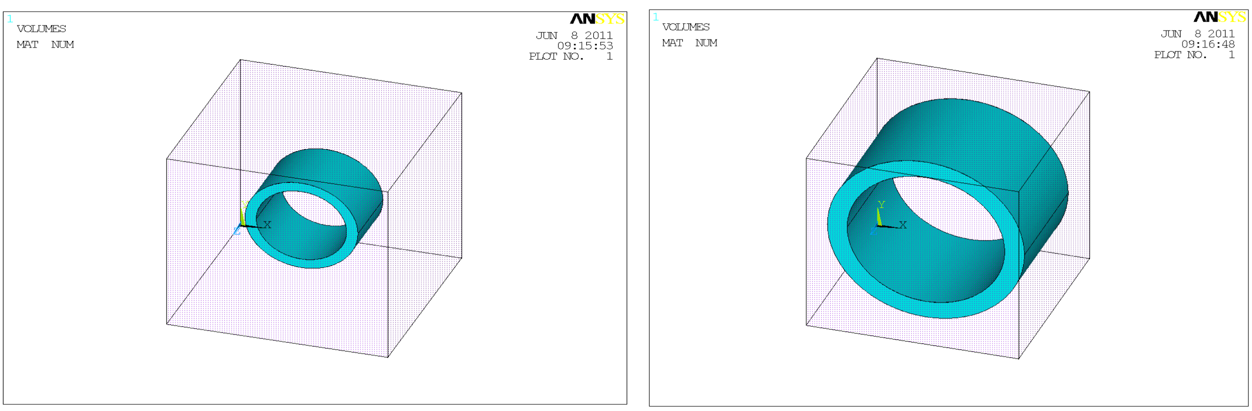
For all non-zero coefficients the effective coefficients were calculated with the numerical homogenization algorithm. Fig. 3 shows calculated effective elastic coefficients over the volume fraction range. It can be seen that the tension coefficients C11, C22 and C33 increases with increasing volume fraction. This is caused by the stiffening influence of the carbon nanotubes [4]. Also, coefficient C21 is increasing with increase of volume of nanotubes which belongs to the transverse plane. But C31 and C32 keep nearly constant which couple longitudinal direction and transverse plane. The transversely isotropy can also be noticed by equality of C11=C22 and C31=C32.

All shear coefficients increases with increasing of volume fraction. C44 and C55 are equal due to transversely isotropy and vary nearly linearly. Effective piezoelectric coefficients are shown in Fig. 4. The coefficients e13 and e23 are equal due to transversaly isotropy and decreases with increasing of volume fraction. The coefficients e33, e51 and e42 can be considered as zero because they are very small compared to e13 and e23. The reason is that PVDF have a very thin film character and nearly no piezoelectric effect in x3 direction which can be seen in zero values of these coefficients in its material constants [5, 6].

Fig. 5 shows effective dielectric coefficients. All increase with increasing volume fraction. This behavior is based on a higher dielectric constant for the carbon nanotubes [13]. k11 and k22 are equal due to transversaly isotropy and k33 is slightly higher. The coefficients are changes very linearly with the variation of volume fraction.

Table 1. Material properties of the constituent phases [5]

Material	Dimension	Young's modulus	Poisson's ratio	Dielectric constant, F/m	Piezoelectric constant, C/m^2
CNT	Length-100 nm Radius-75nm	1000	0.3	0.1327*10e-9	-
PDVF	-	2	0.3	0.1067*10e-9	0.046



(a) (b)

Figure 2. Unit cell models (a) 2.5 % volume fraction and (b) 15 % volume fraction

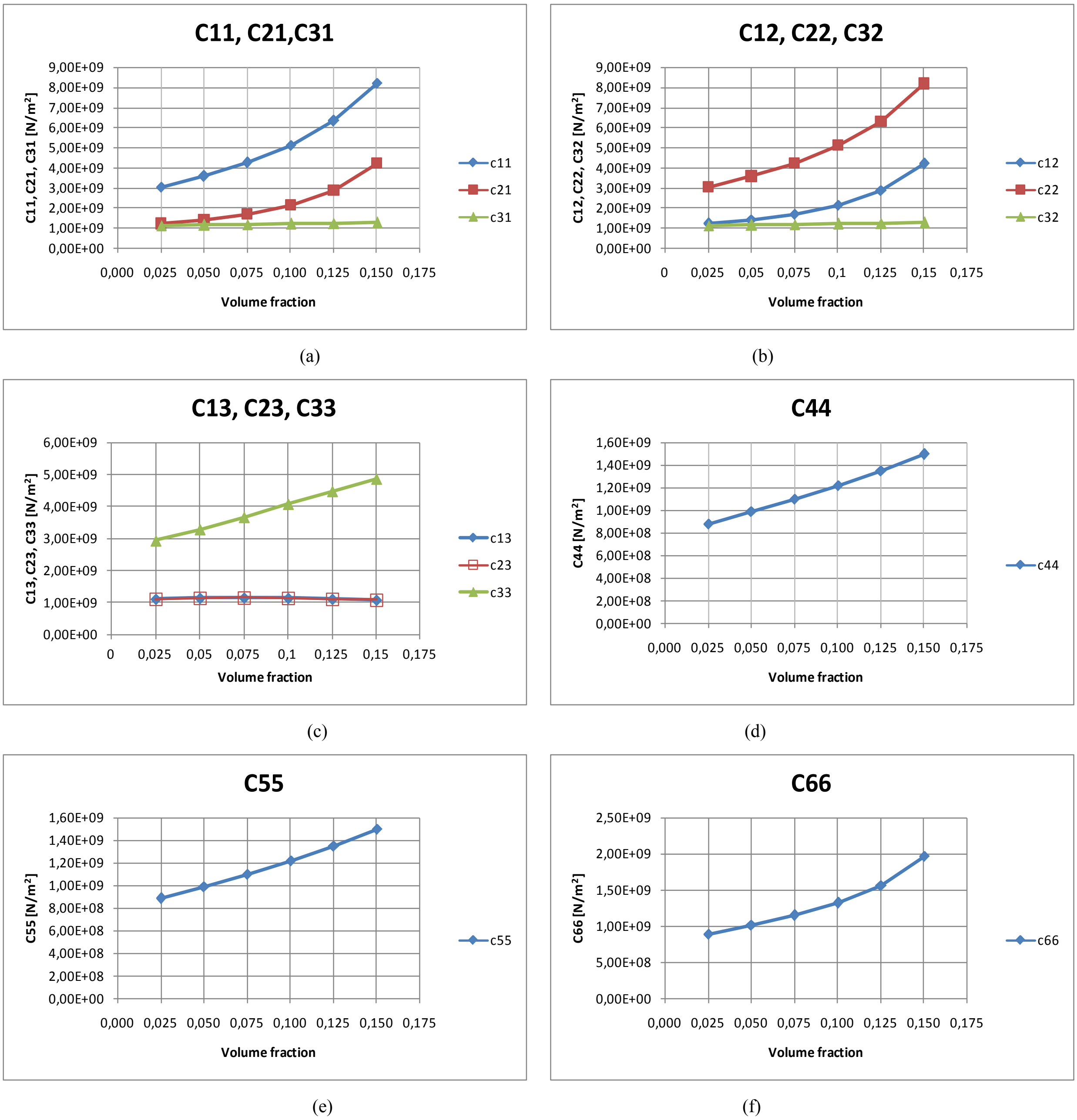
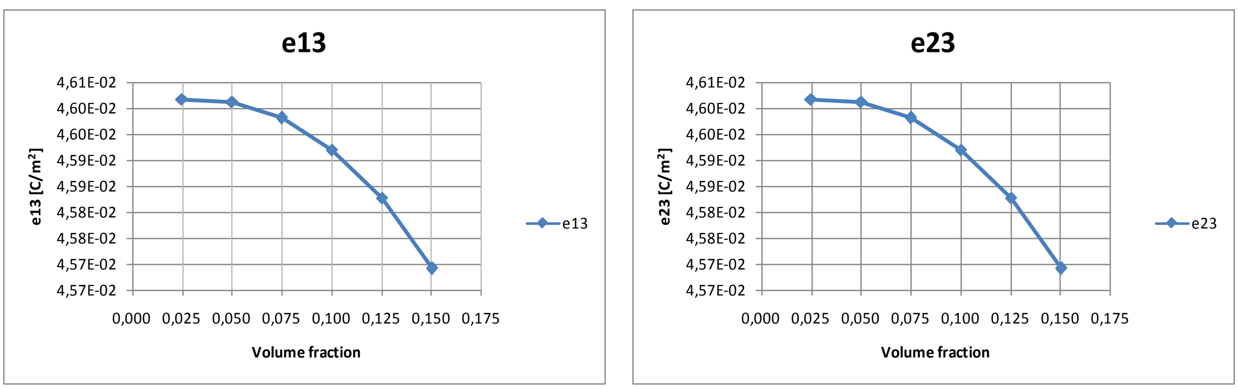
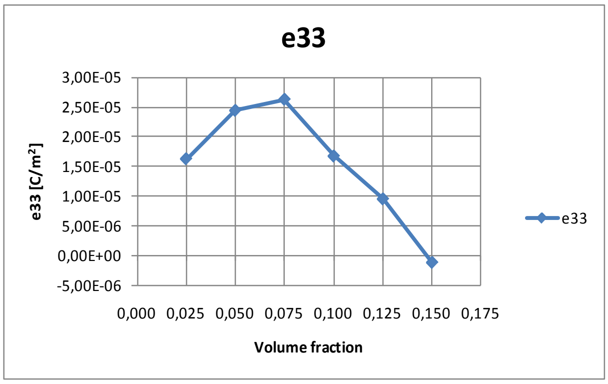


Figure 3. Variation of effective elastic coefficients, (a) C11, C21, C31, (b) C12, C22, C32, (c) C13, C23, C33, (d) C44 (e) C55 and (f) C66 versus volume fraction



(a) (b)



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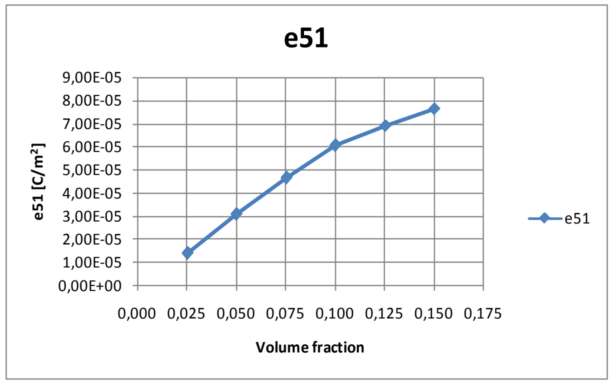

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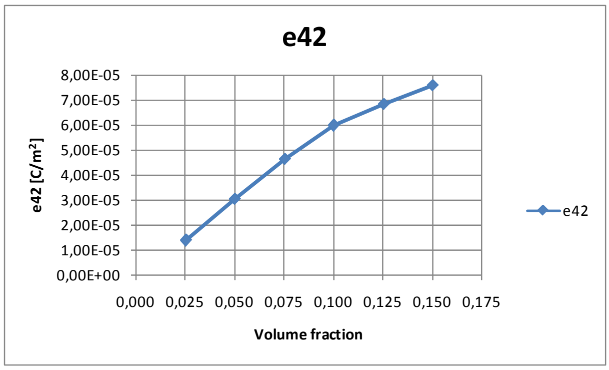
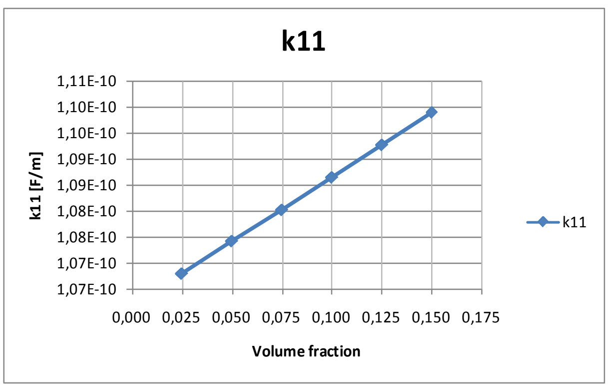
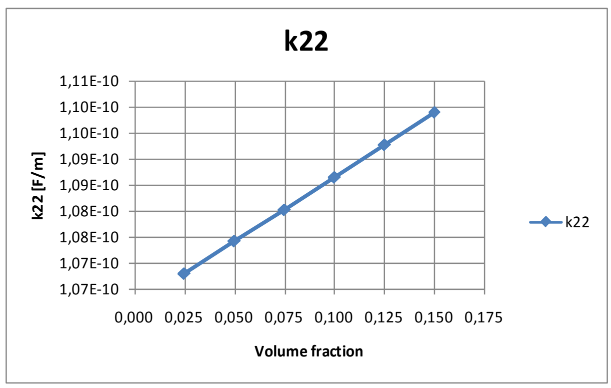


(e)

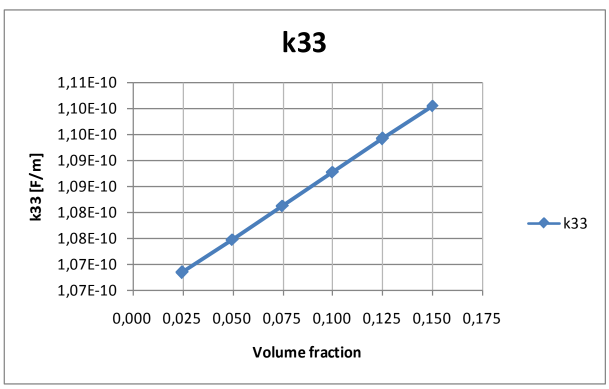
Figure 4. Variation of effective piezoelectric coefficients, (a) e13, (b) e23, (c) e33, (d) e51 and (e) e42 versus volume fraction



(a)



(b)



(c)

Figure 5. Variation of effective dielectric coefficients, (a) k11, (b) k22, and (c) k33 versus volume fraction

4. Conclusions

The investigations deal with calculations of effective material properties for a piezoelectric composite using a numerical homogenization technique with finite element method. Here especially carbon nanotubes are embedded in a piezoelectric matrix of PVDF. The results show the overall behavior of the composite for a regular arrangement of CNTs, aligned in one direction and square pattern. One main challenge in this investigation is find realistic material properties of the component.

It has also been observed that the properties also depend on different parameters like frequency, volume of CNTs in the composites etc. Furthermore the dispersion of the nanotubes can be an important factor.

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