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The mechanical properties investigation of the CNT doped YBCO high temperature superconductor with ANSYS finite element software

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Abstract

In this work we simulated the representative volume element (RVE) of carbon nanotube (CNT) which is surrounded by high temperature superconductor (YBCO) by using ANSYS finite element software. First we considered perfect model (for YBCO and CNT) and investigated the effect of radius, length, and the number of nanotube in Young's modulus of the YBCO by applying force on RVE. Then, a third region an interphase between CNT and YBCO were considered, the Young's modulus of which is between CNT and YBCO. It is demonstrated that there is a critical radius around 6 nm for the CNT and by applying the CNT with a radius smaller than 6 nm, the Young's modulus of the YBCO increases. Also, by increasing the number of the CNTs with radius smaller than 6nm, the Young's modulus and strength of the matrix (YBCO) increases. According to the non-linear analysis, the Young's modulus of the CNT doped YBCO matrix is increased 20-22% more than the undoped YBCO sample.

***Keywords**:* CNT; Young's modulus; YBCO; RVE

1. Introduction

Carbon nanotubes (CNTs) were discovered in 1991 by Iijima (1991). They are considered as a new generation of material possessing special mechanical, thermal, and electrical properties (Dai, 2002; Kang and Heung, 2006; Salvetat and Rubio, 2002; Lau et al. 2006). The applications of the CNTs, especially in the form of composite materials, i.e. CNTs reinforced polymer, have received great attention and interest in recent years. The CNTs have particular mechanical properties such as: high tensile strength and Young's modulus.

The results show that the CNTs have a broad variation of the Young's modulus ranging from 4 to 200 TPa (Fereidoon, 2008). Since applying the CNT to the matrix increases the strength and stiffness of the composite, the CNTs can be used as a reinforcing material in nanocomposites (Thostenson et al., 2001; Lau and Hui, 2002). By applying only 1wt% CNT to the matrix, the stiffness of the matrix can increase about 36%-46% (Qian et al. 2000). Modeling of mechanical properties of nanostructures in theoretical studies is becoming more common when experimental methods faced many professional challenges (Krishnan et al. 1998). Finite element model based on a modified Morse potential has led to simulate graphene and the structural properties of the CNTs (Meo and Rossi, 2006). Description of the interaction between the CNT and the matrix is of great importance in analysis of the CNT reinforced composites, as several models have been developed in this regard (Pour Akbar Saffar and Jamil Pour, 2008). In this work, in order to determine the Young's modulus of a RVE (the CNT and the YBCO matrix), we have designed two models; one with a perfect bond between CNT and matrix and another one with interphase between CNT and matrix.

Carbon nanotubes which are different in shape and size are dispersed in a matrix to form the nanocomposites. They can be single-wall or multi-wall with different length and diameters (Liu and Chen, 2003). The length can be changed up to several micrometers, also they can be straight, twisted, curled, or in the form of ropes (Schadler et al. 1998). Furthermore the arrangement of the CNTs in the matrix can be random. All these factors make the simulations of the CNT-based composites extremely difficult. In the RVE approach, a single (or multiple) nanotube(s) with surrounding matrix material is modeled with properly applied boundary and interface conditions to calculate the effects of the surrounding materials on Young's modulus. Numerical methods, such as finite element method (FEM), boundary element method (Chen and Liu, 2001), or mesh free method (Qian et al. 2001) can be applied to analyze the mechanical reaction of these RVEs under different

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loading conditions. Considering the interphases between CNTs and matrix can make the calculations more accurate and shows the interaction between CNT and matrix (Liu, 2000). In this research, two situations are assumed in order to investigate the Young's modulus of the RVE. In the first situation, the perfect bonding between the CNT and the matrix in the RVE model is considered and in the second situation a third region as an interphase between the CNT and the matrix is also simulated. Three nanoscale RVE (Fig. 1) based on the 3-D elasticity theory have been proposed in Liu et.al's research to study the CNT-based composites (2002).

These RVEs can be used to study the interactions of a CNT with the matrix, such as the load transfer mechanism and stress distributions along the interfaces (Liu and Chen, 2002), or to evaluate the effective material properties of the CNT-based composites.

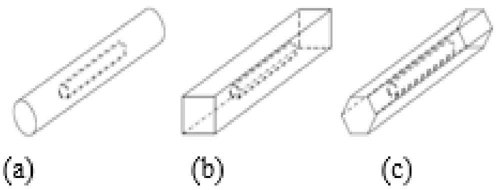

Fig. 1. (a) Cylindrical RVE (b) Square RVE (c) Hexagonal RVE

In this work for evaluation of the effective properties of the CNT-based YBCO high temperature superconductor, square RVEs (Fig. 1(b) was assumed. The Young's modulus of the matrix is also calculated by changing the volume fraction, length, and diameter of the CNT in the axial direction.

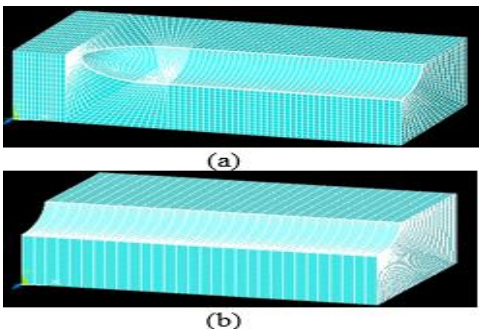

Fig. 2. Meshed model by using finite element method for a) short CNT b) long CNT surrounded by YBCO in a perfect situation

Figure 2 shows the RVE simulation model in which the RVE consists of a single-wall carbon nanotube (a: short CNT b: long CNT) surrounded by YBCO high temperature superconductor. The 8-node tetrahedral element has been used for modeling CNT and YBCO (Fereidoon, 2008).

Several values for Young's modulus and thickness of the carbon nanotubes have been reported, but the result of nanotube's thickness cross to the Young's modulus has been almost constant in all reports (Hosseini Kordkheili and Moshrefzadeh-Sani, 2013). This amount is approximately 0.34 kN/m. Therefore, the thickness of the nanotube was assumed 0.34 nm and its Young's modulus 1000 GPa.

Table 1. The elastic constants used in the finite element software

	Young's Modulus (GPa)	Poisson's Ratio
CNT	1000 (Liu and Chen, 2003)	0.3
YBCO	110 (Toparli et al. 2011)	0.15
CNT in our work	1000	0.3
YBCO in our work	110	0.15

Young's modulus and Poisson's ratio of the CNT and YBCO which have been used in this work, are given in Table1 (Liu and Chen, 2003; Toparli et al. 2011). For using ANSYS finite element software, we applied these two ratios as the inputs.

The relations between Poisson's ratio and Young's modulus with strain are shown in equations 1 and 2.

$$\upsilon = -\frac{d\varepsilon_{trans}}{d\varepsilon_{axial}} = -\frac{d\varepsilon_y}{d\varepsilon_x} = -\frac{d\varepsilon_z}{d\varepsilon_x} \quad (1)$$

$$E = \frac{\sigma}{\varepsilon} \quad (2)$$

where υ is Poisson's ratio, ε_{trans} is transverse strain and ε_{axial} is axial strain. In this regard $d\varepsilon_x=\frac{dx}{x}$, $d\varepsilon_y=\frac{dy}{y}$ and $d\varepsilon_z=\frac{dz}{z}$ are strain on the x, y, z axis respectively. σ and ε are the stress and strain.

In this work, the representative volume element (RVE) consists of the carbon nanotube (CNT) which is surrounded by the high temperature superconductor (YBCO), was simulated by using ANSYS finite element software. ANSYS software is a finite element method which has been used for measuring mechanical properties of composites materials and matrix.

YBCO high temperature superconductor, despite its high Young's modulus, compared to normal composites, is very brittle, so for this reason, carbon nanotube is used to reinforce its stiffness and strength. The aim of this modeling is to investigate the effect of the CNT in the Young's modulus of the YBCO high temperature superconductor as a matrix. To our knowledge, there is no report on improvement of YBCO mechanical properties using CNT doping.

2. Results and discussion

2.1. Short CNT

The RVE elastic response was studied to uniform load along the axis of the CNT. There are many reports about the variation of nanotube's Young's modulus with the radius. Chunyu Li et al (2003) examined Young's modulus of the nanotube by increasing its diameter and found that Young's modulus of CNT increases with its diameter. They found an optimum diameter around 1 nm. Tserpes et al (2005) investigated the Young's modulus of different nanotubes with 0.34 nm thickness and variation of the diameter between 0.5 and 3 nm. They found that the Young's modulus of the nanotubes increased with increasing diameter, but this increase was not constant.

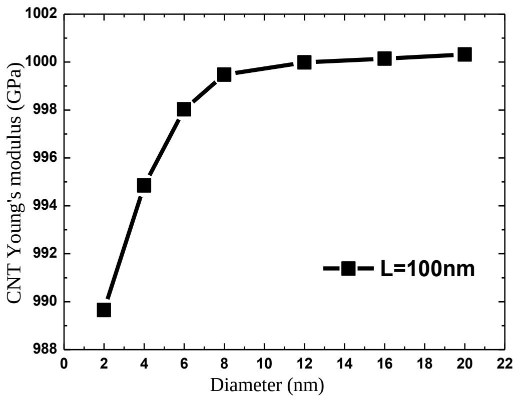

Fig. 3. CNT Young's modulus versus its diameter

In our research, we have studied the Young's modulus of the CNT with 0.34 nm thickness and 100 nm lengths. Result of Young's modulus variations versus the CNT diameter is shown in Fig. 3.The CNT Young's modulus increases with increasing of the CNT diameter. The slope of the curve increases sharply below 8nm and for the diameter higher than 8nm, Young's modulus increases slowly.

In fact, the carbon nanotubes are rolled up graphene sheets. When the CNT's diameter is small, the curvature of C-C bond increases and the stiffness (K) of the CNT decreases which is related to the Young's modulus (E) of the CNT through the equation 3.

$$K = \frac{EA}{L} \quad (3)$$

Also, we modeled a nanotube with the above specifications in a matrix (YBCO). For modeling at first we removed the volume amount of a nanotube with certain radius (5nm) and length (100 nm) from the YBCO matrix and then loaded it. We found that the Young's modulus with the value 110 GPa for the pure YBCO reduced to 108.23 GPa for the matrix (YBCO), and with placing the nanotube with the same radius and length in the empty place the RVE Young's modulus increased to 112.35 GPa. The modeling results for different volume fraction and different CNT radiuses are shown in Fig. 4.

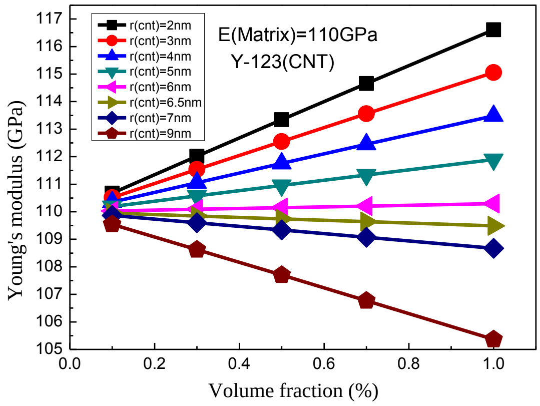

Fig. 4. RVE Young's modulus versus volume fraction

We found that there is a critical radius for the CNT which strengthen the YBCO matrix which is 6 nm for our simulations. As it is shown in Fig. 4, for the CNTs radius bigger than this critical radius, applying CNT to the matrix decreases the Young's modulus of the matrix and for smaller radius it strengthens the matrix.

Stiffness is directly related to the Young's modulus, if we consider the stiffness of the CNT is equal to the stiffness of the YBCO, then we can find the critical radius of the CNT that strengthens the matrix from the equation shown below:

$$K_{CNT} = K_{YBCO} \quad , \quad \frac{2\pi R t E_{CNT}}{L} = \frac{\pi R^2 E_{YBCO}}{L} \quad (4)$$

According to the simulations and equation 4, CNT with radius 6 nm in RVE, introduce critical radius for the RVE Young's modulus. In this case if the CNT with a radius smaller than 6 nm applies to the matrix, the Young's modulus of the RVE is reinforced and with a radius bigger than 6 nm the Young's modulus of the RVE is weakened. So the CNT with 6nm radius can be introduced as a critical CNT for this matrix. Also variation in the length of the nanotubes can change the matrix Young's modulus (Pour Akbar Saffar and Jamil Pour, 2008). We examined the model for 25-36 nm lengths of nanotubes, and the results are shown in Fig. 5.

Figure 5 shows linear behavior of the matrix Young's modulus versus the CNT lengths. For constant dimensions of the matrix and a constant radius of the nanotube smaller than the critical radius by increasing the length of the CNT, RVE Young's modulus increases. The Young's modulus of the RVE for the CNTs radius bigger than the critical radius by increasing the length of the CNT, the RVE Young's modulus decreases. By using the CNT with radius smaller than the critical radius, Young's modulus of the RVE increases, and if the length of this CNT increases due to increasing the volume, Young's modulus also increases. By using the CNT with radius bigger than the critical radius, the Young's modulus of the RVE decreases.

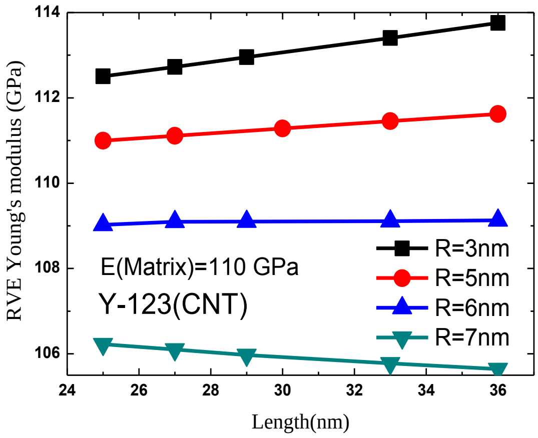

Fig. 5. RVE Young's modulus versus the CNT length

Radius of the CNT has a direct effect on the RVE Young's modulus. Fig. 6 shows the effect of two CNTs which are parallel to each other in the matrix.

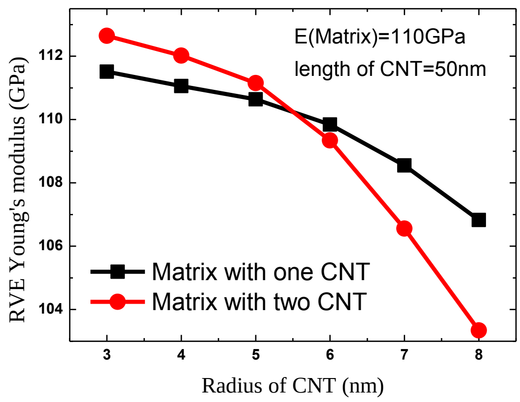

Fig. 6. RVE Young's modulus versus CNT radius

In this model we assumed constant dimension for the matrix (18*18*100 nm^3) and constant length for the nanotube (50 nm).

As it is shown in Fig. 6, by changing the radius of the nanotube from 3 nm to 8 nm, Young's modulus of the RVE decreases dramatically and we found that by increasing the number of the CNTs in the matrix with radius smaller than the critical radius, the RVE Young's modulus increases and by increasing the number of the CNTs with radius bigger than the critical radius the RVE Young's modulus decreases. Also, the RVE Young's modulus for double CNTs with radius higher than the critical radius is smaller than for one CNT.

We conclude that increasing the CNT number from one to two, the Young's modulus of the RVE increases for the radiuses smaller than the critical radius. Therefore, by applying two CNTs with radius smaller than the 6 nm in the matrix with constant dimensions, the RVE is amplified. Also, the results of Fig. 6 confirm the Fig. 4 results.

In the following, we considered interphase region between the CNT and the matrix. It was found that interphase with different Young's Modulus changes the RVE Young's modulus. In this work three different Young's Modulus were considered for the interphase (332.5, 555, 777.5 GPa). These values are the average Young's modulus of the matrix and the CNT and one of them is greater and the other is smaller than the average Young's modulus of the matrix and the CNT. Results show that by increasing the Young's modulus of the interphase, the RVE Young's modulus increases which agrees with other research work (Hu et al., 2005; Achenbach and Zhu, 1989). Liu and et al (2000) reported that the thickness of the interphase affects on the RVE Young's Modulus with volume fraction more than 50% in BEM method. We simulated 3 RVE with 1% volume fraction and different thickness for the interphase 0.2, 0.4, and 0.6nm and observed the RVE Young's modulus increases by increasing the interphase thickness.

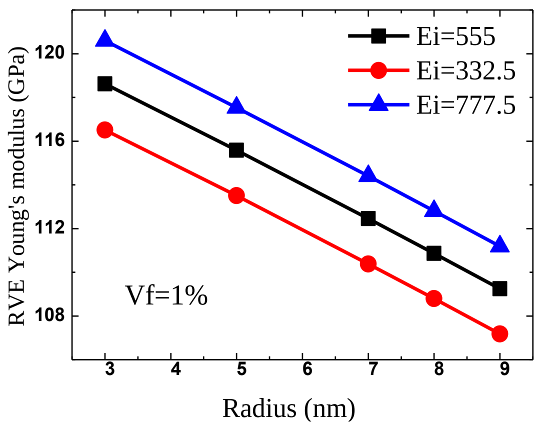

Fig. 7. RVE Young's modulus versus CNT radius for constant interphase thickness

Figure 7 shows decrease of the RVE Young's modulus with increase of the CNT radius while we considered the interphase with different Young's modulus and 0.4 nm thickness between the matrix and the CNT. Masud et al (2009) by using finite element method and considering constant radius for CNT reported Young's modulus of RVE with different matrix increases with increasing Young's modulus of interphase.

2.2. Long CNT

In the previous section the RVE was simulated with short CNT and its Young's modulus investigated and in this section we considered RVE with long CNT. Figure 8 shows the results of this simulation for two RVE with different CNT radius (3 and 5 nm).It is shown that by increasing radius of the long CNT and its volume fraction, Young's modulus of the RVE increases. Increase of the RVE Young's modulus by increasing the CNT's radius depends on the cross sectional area of the CNT in the matrix. Joshi et al (2010) reported similar results that confirm our work.

Composite stiffness can be predicted by using a micro-mechanics approach that nominates the rule of mixtures by assumptions like the CNTs are uniformly distributed throughout the matrix and perfect bonding between CNTs and matrix.

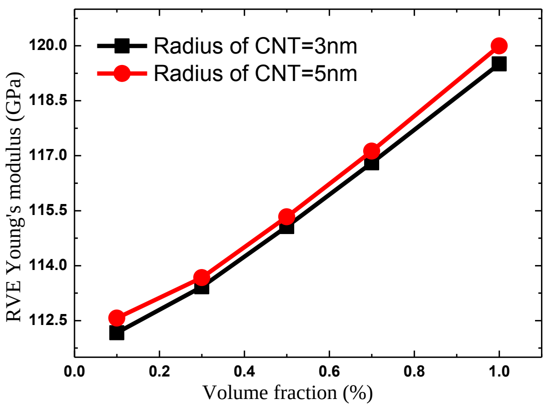

Fig. 8. RVE Young's modulus with long CNT versus volume fraction

The matrix is free of the voids. We apply this approach for the RVE with the long CNT and can be written as follow: (Liu and Chen, 2003).

$$E_c = E_f V_e + E_m(1 - V_e) \quad (5)$$

Where E_c, E_f, E_m is the Young's modulus of the composite, CNT and matrix respectively and V_e is volume fraction of the CNT and can be written as follows:

$$V_e = V_f/(V_f + V_m) \quad (6)$$

where V_f and V_m is volume of the CNT and the matrix respectively. We considered 1% for the RVE volume fraction which consists of the CNT with a radius smaller than critical radius and obtained the RVE Young's modulus 118.9 GPa. By comparing this result with the result of the finite element method we found that its error is around 0.9%, which is in good agreement.

2.3. Non-linear analysis

Up to now we assumed linear behavior for our CNT in the matrix. Now we can consider non-linear behavior of CNT. Non-linear behavior of the CNTs depends on the interatomic potential of the C-C in the CNTs structure. So stress-strain curve of the CNTs is non-linear but it is important that the CNTs behave linear up to 5% strain (Shokrieh and Rafiee, 2010).In the previous sections we assumed linear behavior for the CNT and YBCO but in this section we consider non-linear behavior for the CNT. Different results have been reported in literature for strain at failure point of the CNTs (Yu et al., 2000; Belytschko et al., 2002; Xiao et al. 2005). It changes from 10 to 23% and strain at failure point for YBCO is 0.2% (Vipulanandan and Salib, 1995).

Stress-strain curves for two different RVE consisting of the short and long CNT are shown in Fig. 9 and Fig. 10, respectively. The slope of the stress-strain curve shows the Young's modulus and it is given by equation 2. Figure 9 shows decreasing slope of curves by increasing radiuses of the CNT, therefore the

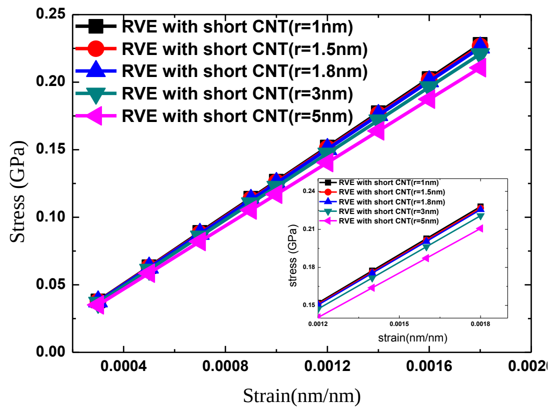

Fig. 9. Stress- strain curve of RVE with short CNT. The inset is stress-strain curve in the range of $0.12*10^{-2}$-$0.18*10^{-2}$

Young's modulus of the RVE decreases by increasing radius of the CNT and it confirms all the linear analysis results in short CNT and long CNT sections. Figure 10 shows the stress versus strain for long CNT.

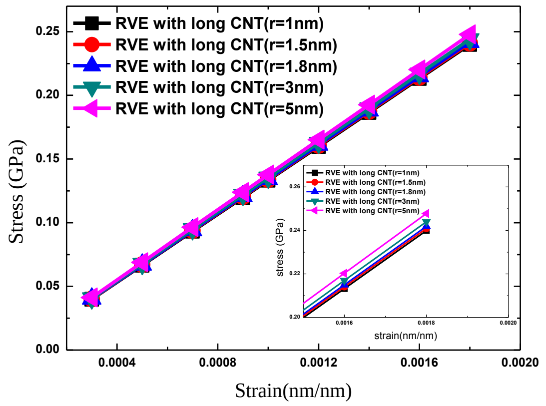

Fig. 10. Stress- strain curve of RVE with long CNT. The inset is stress-strain curve in the range of $0.15*10^{-2}$-$0.18*10^{-2}$

According to the results shown in Fig. 10, RVE of Young's modulus increase by increasing the CNT radius which confirms linear analysis of the RVE with long CNT. We found linear behavior for RVE in both Fig. 9 and 10 in the range of smaller than the YBCO failure strain which is 0.2% and that CNT behaves linearly in this range.

The Young's modulus of the CNT doped YBCO obtained from the curves slope shows, 20-22% increase with respect to the pure YBCO.

Therefore according to our results in this simulation and previous experimental results which have already been reported for the CNT doped YBCO high temperature superconductor (Dadras et al., 2010; Dadras et al. 2009), It can be concluded that the CNT doping is a perfect choice for both electrical and mechanical optimization of this superconductor compound.

3. Conclusions

According to our research it was found that the Young's modulus of the SWCNT depends on its radius and Young's modulus increase with increasing its radius. Applying the CNT into the YBCO matrix, Young's modulus of the RVE varies. There is a critical radius around 6 nm for the CNT that with a radius smaller than 6 nm, the Young's modulus of the RVE increases and with a radius bigger than 6nm, the RVE Young's modulus decreases.

Also we investigated variations of CNT length effect. We found that when radius is less than 6 nm, with increasing CNT length the RVE Young's modulus increases and with radius higher than 6 nm with increasing CNT length the RVE Young's modulus decreases.

According to the non-linear analysis, the RVE Young's modulus with the long CNT increases by increasing the radius of the CNT. The Young's modulus of the CNT doped into YBCO is increased 20-22% more than pure YBCO.

For future work, we propose that CNT doping is a perfect candidate for both electrical and mechanical optimization of YBCO superconductor compound.

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