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Numerical Simulations on Piezoresistivity of CNT/Polymer Based Nanocomposites

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Abstract: In this work, we propose a 3 dimensional (3D) numerical model to predict the piezoresistivity behaviors of a nanocomposite material made from an insulating polymer filled by carbon nanotubes (CNTs). This material is very hopeful for its application in highly sensitive strain sensor by measuring its piezoresistivity, i.e., the ratio of resistance change versus applied strain. In this numerical approach, a 3D resistor network model is firstly proposed to predict the electrical conductivity of the nanocomposite with a large amount of randomly dispersed CNTs under the zero strain state. By focusing on the fact that the piezoresistivity of the nanocomposite sensor is largely influenced by the tunneling effects among neighboring CNTs, we modify this 3D resistor network model by adding the tunneling resistance between those neighboring CNTs within the cut-off distance of tunneling effect, i.e., 1.0 nm in this study. The predicted electrical conductivity by this modified 3D resistor network model is verified experimentally. Furthermore, to analyze the piezoresistivity of the nanocomposite sensor under various strain levels, this modified 3D resistor network model is further combined with a fiber reorientation model, which is used to track the orientation and network change of rigid-body CNTs in the nanocomposite under applied strain. This combined model is employed to predict the piezoresistivity of the nanocomposite iteratively corresponding to various strain levels with the experimental verifications. Some key parameters, which control the piezoresistivity behavior, such as, cross-sectional area of tunnel current, height of barrier, orientation of CNTs, and electrical conductivity of CNTs and other nanofillers, are systematically investigated. The obtained results are very valuable, which can provide guidance for designing the strain sensor of this nanocomposite with enhanced sensitivity.

Keywords: carbon nanotube, nanocomposite, piezoresistivity, tunneling effect.

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1 Introduction

Carbon nanotubes (CNTs) of high aspect ratio possess excellent electrical conductivity. Therefore, with a small amount of CNTs, which are dispersed in insulating polymers, it is possible to produce nanocomposites with high electrical conductivity. This kind of conductive CNT/polymer nanocomposite can be applied to various fields, such as highly sensitive strain sensors, electromagnetic interference materials, etc. In the field of strain sensor made from this kind of new materials, for instance, it has been confirmed that the conductance of a CNT could be dramatically changed by introduction of strain using atomic force microscopy (AFM), as a consequence of the structural change under the effect of mechanical strain, such as the change of chirality in a single-walled carbon nanotube (SWCNT) [Tombler *et al.* (2000)]. Due to this piezoresistivity property of CNTs, it was predicted that integrating CNTs into polymers would open up a whole range of smart structure applications [Ajayan and Zhou (2001); Baughman, Sakhidov and deer Heer (2002)]. In particular, great interest has recently been aroused in building strain sensors with CNTs [Frogley, Zhao and Wagner (2002); Dharap *et al.* (2004); Li *et al.* (2004); Kang *et al.* (2006); Halary *et al.* (2004); Ramaratnam and Jalili (2006); Hu, Karube, Arai *et al.* (2008); Hu *et al.* (2010); Pham *et al.* (2008)]. Generally, CNTs are Raman active, and are able to be blended with a polymer to make a strain sensor provided a relationship between mechanical strain and Raman band shift can be calibrated [Frogley, Zhao and Wagner (2002)]. Obviously, implementation of complex equipment in this technique remains a technical challenge, especially for a field application. Alternatively, resistance-type strain sensors have been increasingly used to measure the strains on the surfaces of a structure. To this end, two types of strain sensors have been developed, i.e., SWCNT buckypaper sensors [Dharap *et al.* (2004); Li *et al.* (2004); Kang *et al.* (2006)] and sensors made from CNT/polymer nanocomposites, where SWCNT or multi-walled carbon nanotube (MWCNT) was used [Kang *et al.* (2006); Halary *et al.* (2004); Ramaratnam and Jalili (2006); Hu, Karube, Arai *et al.* (2008); Hu *et al.* (2010); Pham *et al.* (2008)]. As compared to conventional sensors, higher sensitivity has been observed in these novel sensors, at least at a macro-scale [Kang *et al.* (2006); Hu, Karube, Arai *et al.* (2008); Hu *et al.* (2010); Pham *et al.* (2008)]. Moreover, linear piezoresistivity has been identified in these sensors within very small strain range, e.g., 200 μs or 1000 μs [Kang *et al.* (2006); Ramaratnam and Jalili (2006)], whereas the nonlinear piezoresistivity has also been reported for a quite large strain range, e.g., 6000 μs. [Halary *et al.* (2004); Hu, Karube, Arai *et al.* (2008); Hu *et al.* (2010)]. In spite of these promising results, the fundamental understanding of piezoresistivity behavior in a CNT/polymer nanocomposite is still lacking, largely due to the less effort being put into theoretical and numerical investigations on the piezoresistivity behavior in these materials.

In this work, based on our previous numerical model built up from 3D statistical resistor network model [Hu, Masuda, Yan *et al.* (2008)] for predicting the electrical conductivity of nanocomposites, to investigate piezoresistivity behavior which underpins the working principle of these sensors, we propose an improved 3D statistical resistor network model by which the tunneling effect among randomly distributed CNTs in a polymer matrix can be evaluated. The change of CNT networks in the polymer under a given strain is predicted using a fiber reorientation model. Then, the resistance change of the nanocomposites caused by the applied strain is estimated by using the 3D resistor network model and the fiber reorientation model in an iterative way. The predicted electrical conductivity and piezoresistivity of nanocomposite are verified using our previous experimental data [Hu, Karube, Arai *et al.* (2008); Hu, Masuda, Yamamoto *et al.* (2008); Hu *et al.* (2010)]. Moreover, the influences of various parameters, such as, cross-sectional area of tunnel current, height of barrier, orientation of CNTs, and electrical conductivity of CNTs and other nanofillers, on the piezoresistivity of nanocomposites are systematically investigated.

2 Computational model

To predict the electrical conductivity of the nanocomposite, a 3D resistor network that contains randomly distributed CNTs in the polymer has been constructed. So far, the resistor network model has been well documented [Balberg and Binenbaum (1985); Kirkpatrick (1971); Kirkpatrick (1973)]. However, because it is a troublesome and large-scale computational work, numerical studies based on a fully 3D statistical resistor network model, even for predicting the electrical conductivity of conventional electronic composites with filler materials such as short carbon fibers, have been very limited. Most of these models have been based on the RC (resistor-capacitor) from a simulated microstructure. For convenience, in this research, the electrical conductive paths in the matrix phase are completely neglected. Moreover, as shown in Fig. 1 for a fractured surface of a sample with a 2.0 wt% MWCNT loading [Hu *et al.* (2010)], there is no obvious aggregation in our various specimens using different fabrication processes for this nanocomposite. Therefore, aggregation of CNTs is neglected in this study. The CNTs are considered as cylinders of length L and diameter D. For the ideal state of uniformly dispersed straight CNTs in matrix as shown in Fig. 2, the simulations are carried out using the following procedure:

First, a 3D unit cell is constructed. The size of the unit cell is varied in order to achieve a stable and converged electrical conductivity of nanocomposites.

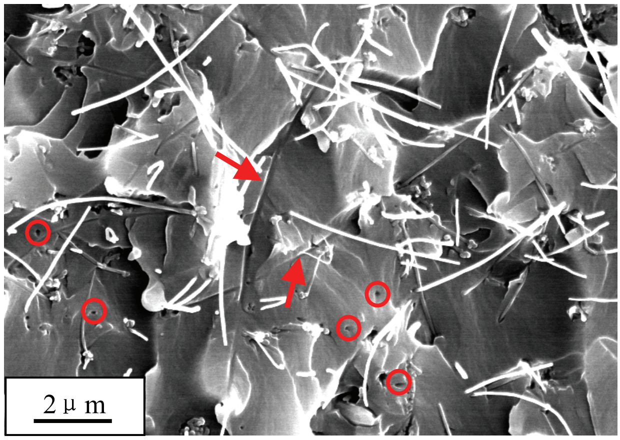

Figure 1: Dispersion state of CNTs and evidence of weak interface between CNTs and polymer matrix

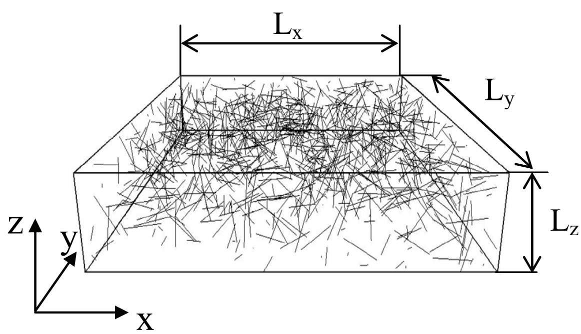

Figure 2: A 3D representative unit cell

Next, CNTs are randomly put (one at a time) into the 3D cube and their orientations in space are chosen randomly as follows:

The coordinates of two ends of a randomly dispersed CNT, i.e., (x_1, y_1, z_1) and (x_2, y_2, z_2) can be set as follows

$$x_1 = rand \times L_x, \quad y_1 = rand \times L_y, \quad z_1 = rand \times L_z \tag{1}$$

$$x_2 = x_1 + L \cdot v_1 \cdot \cos(w_1), \quad y_2 = y_1 + L \cdot v_1 \cdot \sin(w_1), \quad z_2 = z_1 + L \cdot u_1 \tag{2}$$

where L_x, L_y and L_z are the lengths of the 3D element along x, y and z axes, respectively, as shown in Fig. 2, *rand* is a random number located in [0,1], which is uniformly generated. Furthermore, the parameters representing alignment directions of CNTs, i.e., u_1, v_1 and w_1 are expressed as follows:

$$u_1 = 1.0 - 2.0 \times rand, \quad v_1 = \sqrt{1.0 - u_1^2}, \quad w_1 = 2\pi \times rand \tag{3}$$

Some generated CNTs may be partially located outside of the 3D representative cube. In this case, by finding the interactions of these CNTs with the 6 boundary planes of 3D cube, the portions on these CNTs, which are located outside of the 3D cube, are removed automatically and the intersections on the 6 boundary planes are numbered as the ends of these CNTs.

Each time after a new CNT is added into the unit cell, it is checked if it is in contact with one or more of CNTs already present in the unit cell. This is done by determining the minimum distance between the axes of the CNT in question and the axes of the remaining CNTs. In general, the shortest distance d between two skew CNTs can be calculated from the length of common perpendicular to the two axis lines of CNTs. If such distance for two CNTs is smaller than the nanotube diameter (D), the CNTs are considered to be in contact.

When two CNTs are found to be in contact, the intersection is numbered. Until the amount of added CNTs reaches to the required volume fraction of CNTs in the 3D cube and all intersections among CNTs are numbered sequentially to form a global conductive network.

To construct the 3D resistor network model as shown in Fig. 3 (only a 2D model is shown here), for a CNT with two contacting points i and j with neighboring CNTs, the conductance g_{ij} between i and j(the inverse of resistance R_{ij}) can be evaluated as:

$$g_{ij} = \sigma_{CNT} \frac{S_{CNT}}{l_{ij}} \tag{4}$$

where l_{ij} is the length between the points i and j, and σ_{CNT} and S_{CNT} are electrical conductivity and cross-sectional area of the CNT, respectively.

Moreover, unlike the so-called "soft-core" model of fiber [Balberg and Binenbaum (1985); Kirkpatrick (1971); Kirkpatrick (1973)], in the present study, to deal with both tensile and compressive strains, we model CNTs as "hard-core" objects, with the assumption of non-penetration between the CNTs. As shown in Fig. 3, for randomly distributed CNTs in a three-dimensional unit cell, when the distance between two adjacent CNTs is reduced to zero (in contact each other) or to the cutoff

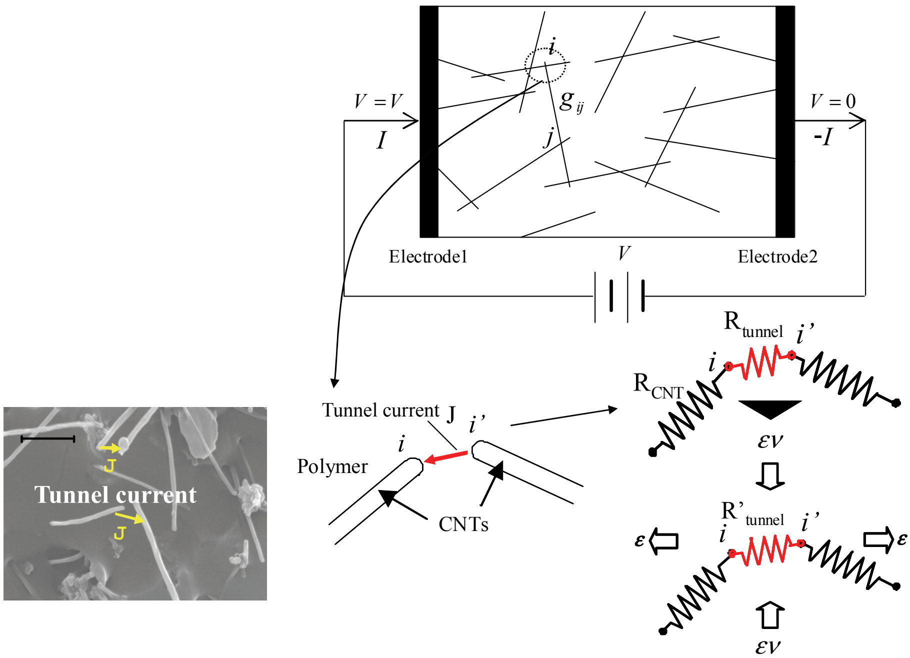

Figure 3: Schematic view of CNT conductive network including tunneling effect

distance, the tunneling effect (resistance) is introduced. For example, at the point i (Fig. 3), if two CNTs are in contact or penetrate to each other, we *intentionally* separate them with a shortest distance of 0.47 nm to avoid further penetration, and then add tunneling resistance R_{tunnel} between them. This operation is very time-consuming for very high CNT loading cases since there may be multiple contact points for one CNT from other neighboring CNTs. For lower CNT loading discussed here, this operation is comparatively simple. The shortest distance (0.47 nm) is determined by matching the conductivity and piezoresistivity predicted numerically with the experimental ones. It is reasonable to set up this shortest distance (0.47 nm) since in general, the equilibrium distance between two independent carbon atomic structures under Lennard–Jones potential or van der Waals force ranges approximately from 0.3 nm to 0.5 nm. Furthermore, it is interesting to see the shortest distance is much lower than the average diameter of the CNTs in the numerical simulations, i.e., 50 nm. At the same point, if two CNTs are not in contact or penetration state, but are located within the cutoff distance, i.e., 1.0 nm, we also introduce the tunneling resistance. Therefore, the distance d between two central lines of two CNTs for introducing the tunneling effect is,$D+d_{min} < d \leq D+d_{max}$, where$d_{min}$, d_{max} and D are set to be 0.47 nm, 1.0 nm and average diameter of CNTs, respectively. The reorientation of CNTs under applied strains is simplified as rigid-body movement, due to the much higher Young's modulus of CNTs compared with a polymer matrix and the very weak interface between CNTs and the matrix [Hu, Karube, Arai *et al.* (2008)]. The resistance change caused by the tunneling effect is schematically shown in Fig. 3. The tunneling resistance between two neighboring CNTs can be approximately estimated as [Simmons (1963)],

$$R_{tunnel} = \frac{V}{AJ} = \frac{h^2 d}{Ae^2\sqrt{2m\lambda}} \exp\left(\frac{4\pi d}{h}\sqrt{2m\lambda}\right) \tag{5}$$

where J is tunneling current density, V the electrical potential difference, e the quantum of electricity, m the mass of electron, h Planck's constant, d the distance between CNTs, λ the height of barrier (for epoxy, 0.5eV$\sim$2.5eV), and A the cross-sectional area of tunnel (the cross-sectional area of CNT is approximately used here).

Based on the well-known matrix representation for a resistor network [Balberg and Binenbaum (1985); Kirkpatrick (1971)] and Kirchhoff's current law, the total current I under an applied voltage can be estimated. This is a large-scale linear system, because the number of CNTs involved in the numerical model is very large, and ranges from several thousands to several tens of thousands depending on the aspect ratio of the CNTs. An iterative equation solver, i.e., the incomplete Cholesky conjugate gradient method (ICCG) has been employed to solve these linear equations for obtaining the total current I. Then the macroscopic electrical conductivity of nanocomposites can be evaluated by the Ohm's law.

In this work, the piezoresistivity is completely evaluated via numerical simulation, incorporating the change of inter-filler distances and possible breakup of conductive networks when subjected to strains. The resistance change of CNTs under elastic strain is ignored since its contribution can be considered to be insignificant under a small strain, as confirmed in the study of SWCNT buckypaper film [Dharap *et al.* (2004)]. Moreover, the experiment used the tip of an AFM to manipulate MWCNTs, revealing that changes in the sample resistance existed, but were very small unless the MWCNTs were fractured [Paulson *et al.* (1999)]. In fact, very limited deformation is expected in the CNTs due to the poor stress transfer from the polymer matrix to these tubes, caused not only by the large elastic mismatch between the CNTs and the polymer but also by the weak interface strength. For instance, the elastic modulus of a CNT (1.0 TPa) is about 300 times higher than the epoxy (2.4 GPa). Figure 1 also shows the complete debonding and pull-out holes of CNTs from the polymer matrix, indicating low interface strength in our nanocomposite. Considering the rigid-body movement of the CNTs, the change of position and orientation of the CNTs under the effects of strain and Poisson's ratio are evaluated using the 3D fiber reorientation model [Taya, Kim and Ono (1998)] based on an affine transformation and the assumption of the incompressibility of the nanocomposite (see Fig. 3). Corresponding to an updated distribution of the CNTs under a prescribed strain, a new network of CNTs can be formed by re-calculating the possible intersections between CNTs and tunneling resistances between CNTs within the cutoff distance. The switch of the intersections of CNTs to possible tunneling effect due to the breakup of CNT contacts and the distance update of pre-existing tunneling effects are modeled. Then, the resistance of the nanocomposite can be re-evaluated using the 3D resistor network in an iterative way.

3 Verifications

To verify the present numerical model, we first estimate the electrical conductivity of CNT/polymer nanocomposites without applied strains. In principle, the electrical conductivity should be independent to the sample volume, such as the size of the unit cell selected for numerical simulation, provided there are sufficient CNTs in the matrix and a stable conductive network is expected to form. To reduce the computation cost, the numerical simulation are conducted in a unit cell with dimensions of 25 μm (length)$\times$25 μm (width)$\times$25 μm (thickness) containing MWCNTs with length of 5 μm (L) and diameter of 50 nm (D) as used in our previous experiments [Hu, Masuda, Yamamoto *et al.* (2008)]. The unit cell has been estimated large enough for an isotropic behavior and numerical convergence [Hu, Masuda, Yan *et al.* (2008), Hu, Masuda, Yamamoto *et al.* (2008)]. The barrier height of epoxy (λ) in Eq. 4 is set as 1.5 eV, and electrical conductivity of CNTs is chosen as 10^4 S/m. The average electrical conductivity predicted from 50 Monte-Carlo simulations using the proposed model is compared with existing experimental and numerical results, as shown in Fig. 4. It can be seen in Fig. 4 that the conductivity predicted by the present model is slightly lower than that in our previous simulation [Hu, Masuda, Yan *et al.* (2008)], at which the tunneling effect was not considered, and the CNTs were assumed in perfect contacting state in the intersection points. On the other hand, good agreement can be observed between the present prediction and the three experimental results [Hu, Masuda, Yamamoto *et al.* (2008), Ono, Aoki and Ogasawara (2006), NCT Co., Ltd. (2004)], conducted by using a same MWCNT (060125-01K) with the same dimensions mentioned previously, which is supplied by Nano Carbon Technologies (NCT) Co., Ltd. in Japan.

Next, we examine the resistance change ratio of sensor due to applied strains, i.e., $\Delta R/R_0$, where R_0 is the initial resistance of sensor. The numerical prediction is

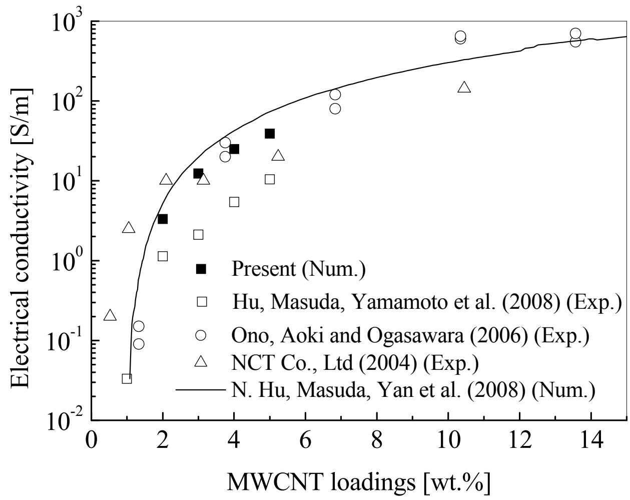

Figure 4: Various results for electrical conductivity of CNT/polymer nanocomposite

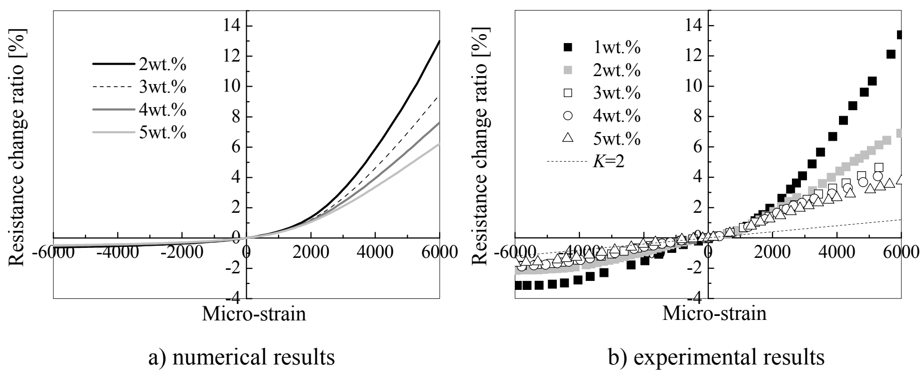

Figure 5: Comparison of numerical and experimental piezoresistivities of strain sensor

shown in Fig. 5(a), together with the experimental results [Hu *et al.* (2010)] in Fig. 5(b). In Fig. 5(b), the resistance change ratio in a traditional strain gauge with a gauge factor K=2 is also included. In these figures, it can be seen that the present numerical simulations can qualitatively catch the main trend of the experimental results, especially under tensile strain. The nonlinear behaviors of numerical and experimental piezoresistivities can be observed clearly. It implies that the tunneling effect plays a very important role in determining the overall performance of the nanocomposites when the CNT loading is low. According to Eq. 4, 1 Å increase of d(the distance between two CNTs) can lead to 10 times lower tunneling current (λ=0.5eV, $A=\pi(D/2)^2$, and D=50nm). From Eq. 5, the tunneling resistance increases exponentially with the average distance d. Approximately, d is assumed to change proportionally to an applied strain. As a result, a nonlinear relationship between the resistance and an applied strain is expected, as shown in Figs. 5(a) and 5(b). Especially for the cases of low CNT loading and higher strains, this nonlinear behavior is more obvious which indicates that the tunneling effect plays a dominant role in these cases. Moreover, similar to some experimental studies [Kang *et al.* (2006); Hu, Karube, Arai *et al.* (2008); Pham *et al.* (2008)], low CNT weight fraction can increase the sensitivity of a sensor. The reason for this phenomenon is that the sensor sensitivity is attributed to the resistance change mainly caused by the breakup of CNT conductive network or tunneling effects. For coarse conductive network, the breakup of a few conductive paths can lead to a huge increase of sensor resistance, which results in the higher sensor sensitivity. Inversely, for dense CNT conductive network, the breakup of a few conductive paths cannot cause a significant change of total sensor resistance. Moreover, from Figs. 5(a) and 5(b), obviously, the resistance change under larger strain can be predicted by our numerical model. The results in Figs. 5(a) and 5(b) validate that the present model can predict the performance of a sensor made from stiff MWCNTs with a large diameter, which are of comparatively straight shape and less aggregates. Furthermore, both in numerical and experimental results, it is interesting to note that the sensor sensitivity in a sensor is much lower when subjected to compressive strain than tensile one. Generally, a sensor is expected to work more efficiently when subjected to tensile strain as the increase of distances between neighboring CNTs is unlimited by considering the contribution of tunneling effects. However, under compressive strain, there is a minimum distance among the CNTs due to the non-penetration restriction applied. As a result, with increase of compressive strain, the sensitivity of a sensor is reduced and finally saturated as shown in Figs. 5(a) and 5(b).

4 Numerical investigations

After verifying the effectiveness of the present numerical model, we investigate the influences of various parameters on piezoresistivity using it. First, by considering Eq. 5, two important parameters are chosen, i.e., λ: the height of barrier, and A: the cross- sectional areas of tunnel. For A, here, the diameter of MWCNTs used in experiments [Hu, Karube, Arai *et al.* (2008); Hu *et al.* (2010); Hu, Masuda, Yamamoto *et al.* (2008)] is used as a standard value. The influence of various

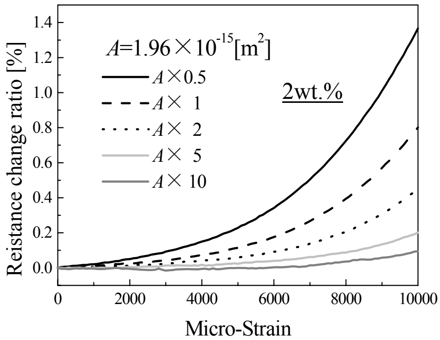

Figure 6: Influence of $\boldsymbol{A}$

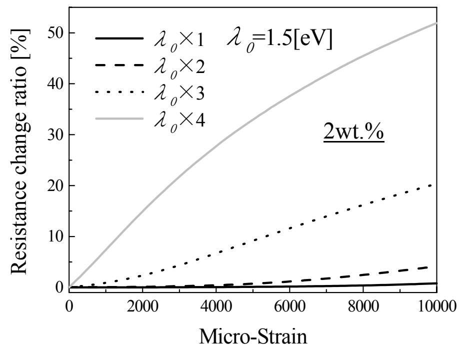

Figure 7: Influence of λ

cross-sectional area of CNTs on piezoresistivity is shown in Fig. 6 when keeping λ to be 1.5 eV and CNT loading to be 2.0 wt.%. Observation of Fig. 6 reveals that with the decrease of the cross-sectional area A of CNTs, the piezoresistivity of the sensor increases remarkably. Next, we keep the cross-sectional area of tunnel as 1.96×10^{-15} m^2 and CNT loading as 2.0 wt.% to investigate the influence of the height of barrier, i.e., λ. As shown in Fig. 7, we can find that with the increase of λ, the piezoresistivity of the sensor increases, which corresponds to the increase of tunneling resistance by viewing Eq. 5. Moreover, by comparing Fig. 7 with Fig. 6, it can be found that the influence of λ. is much more significant than that of A, which highlights the importance of selection of proper polymer with a higher λ. Moreover, it can be found from the present results that the decrease of A or increase of λ leads to the obvious increase of the total initial resistance of sensor, i.e., R_0 due to substantial increase of tunneling resistance in sensor.

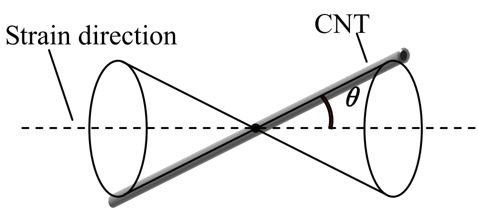

Figure 8: Definition of θ

Another important factor is the orientation of CNTs in matrix, some previous studies [Park *et al.* (2006)] have shown that a parallel alignment of CNTs in matrix

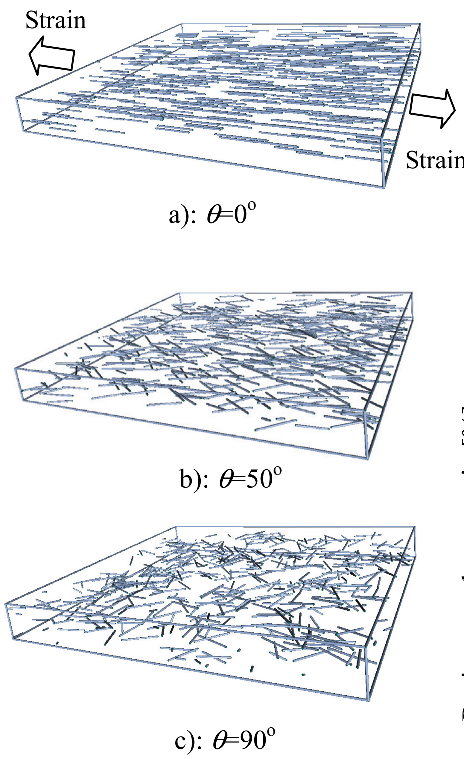

Figure 9: Models for various θ

can help increase the electrical conductivity, and reduce the percolation threshold of nanocomposites. To generate the numerical models with the various CNT orientations, the orientation angle θ of CNTs is defined in Fig. 8. In this figure, the CNT can be randomly orientated within the top angle θ of the cone. When θ =90^o, the numerical model corresponds to that of complete uniform random distribution of CNTs. Three representative numerical models with the different θ are shown in Fig. 9 when CNT loading is equal to 2.0 wt.%. When θ is smaller than 50^o, due to strong numerical instabilities in the ill-conditioned linear system of the resistor network model caused by the incomplete conductive network, we cannot get the piezoresistivity of the sensor. Figure 10 shows the influence of θ on the piezoresistivity of the sensor when CNT loading is equal to 2.0 wt.%. When θ =90^o, the present result agrees with that of a model with complete randomly distributed CNTs very well, which validates the effectiveness of our proposed model. From Fig. 10, we can find that the increase of θ leads to the higher piezoresistivity of the sensor. It means that the state of complete randomly orientated CNTs is desirable,

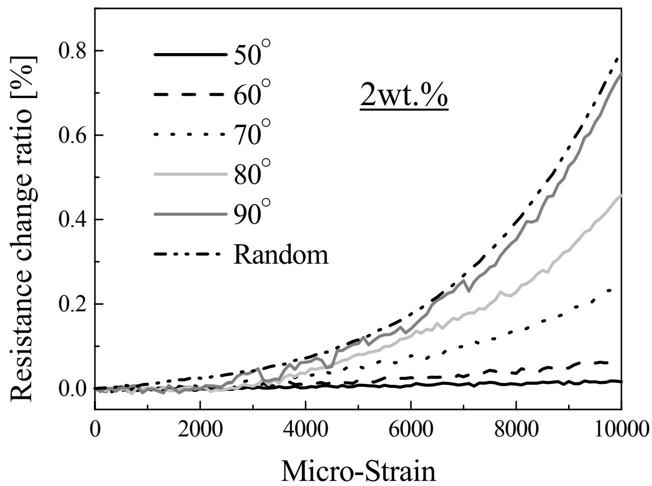

Figure 10: Influence of θ

which was verified in our previous experimental study [Hu *et al.* (2010)], where the higher mixing speed for dispersing CNTs into matrix in the manufacturing process can lead to the higher sensitivity of sensor. By observing Fig. 9(a) for θ=0^o, we can also provide a more clear physical explanation. As shown in this figure, all CNTs are parallel to the strain direction. In this case, the distances among CNTs in the direction vertical to strain direction, which may cause the possible tunneling resistance change, do not vary significantly under tensile or compressive state. Therefore, the tunneling resistance does not change significantly in this case. Inversely, for the case of Fig. 9(c), where CNTs are complete randomly orientated, there are a lot of possible locations where tunneling resistance can be changed due to the applied strain in any in-plane direction. Of course, in this case, the total initial resistance of sensor also increases.

Finally, it might be worthwhile investigating the effect of electrical conductivity of nanofillers on sensor sensitivity. The conductivity of MWCNTs was reported in the ranges of 5×10^3 $\sim5\times10^6$ S/m [de Heer *et al.* (1995); Hobara *et al.* (2004)]. Compared with MWCNTs, much higher conductivities were observed in some recently developed metallic nanowires, e.g., Ag (63×10^6 S/m), Cu (59.6×10^6 S/m) and Au (45.2×10^6 S/m). Therefore, the selection of nanofillers may play an important role in manipulating the sensor sensitivity. To this end, numerical simulation is conducted and the results are shown in Fig. 11. It can be seen that the resistance change ratio increases significantly with the conductivity of the nanofiller. With increase of the conductivity of the filler from 10^3 S/m to 10^6 S/m, the gauge

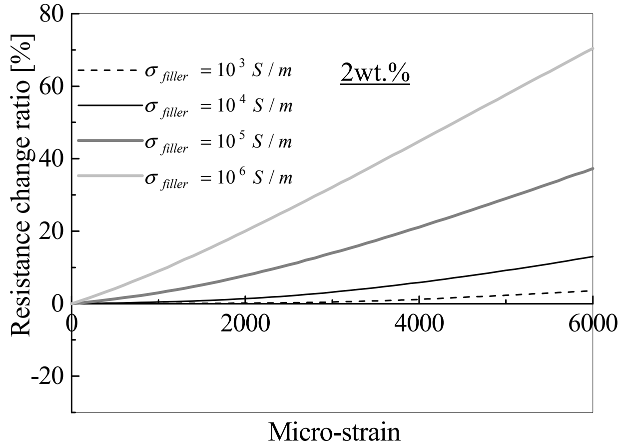

Figure 11: Influence of electrical conductivity of nanofiller on sensor sensitivity

factor corresponding to 6000 $\mu\varepsilon$ tensile strain increases remarkably from 6.0 to 117! In general, the conductivity of nanocomposites increases with the conductivity of fillers added in our previous studies [Hu, Masuda, Yan *et al.* (2008)]. Therefore, this result seems to be inconsistent to the results shown in the previous figures, e.g., Figs. 6, 7 and 10, where the higher total resistance of nanocomposite or higher tunneling resistance in sensor corresponds to higher gauge factor. In fact, the overall resistance of a nanocomposite with CNT networks (Fig. 3) is mainly contributed by the resistance of nanofiller and the tunneling resistance. The resistance of nanofillers decreases with increase of their conductivity, which leads to a higher ratio of the tunneling resistance to the overall resistance of the nanocomposite. In other words, the key to improvement of sensor sensitivity is increase of either tunneling resistance or the ratio of the tunneling resistance to the total resistance, rather than the total resistance itself.

5 Conclusions

In this work, the piezoresistivity behavior of a strain sensor made from a CNT/polymer nanocomposite has been numerically investigated by employing a 3D resistor network model incorporating the tunneling effect of CNTs, which is further combined with a fiber reorientation model. It is found that this model can yield very good results of piezoresistivity of the sensor by comparing with experimental results. We have identified that the tunneling effect plays a key role in the performance of the sensor under small strains. Much higher sensitivity of the sensor can be obtained for lower CNT loadings, which can only form a coarse conductive network. The behavior of the sensor is weakly non-linear due to the tunneling effect. The influence of various factors in the numerical model on the piezoresistivity of the sensor has been investigated numerically. It can be found that the decrease of cross-sectional area of carbon nanotube, i.e., A or the increase of the height of barrier, i.e., λ. determined by polymer type, can lead to the higher sensor sensitivity, and the obvious increase of the total initial resistance of sensor, i.e., R_0 due to substantial increase of tunneling resistance in sensor. However, it is also found that the increase of electrical conductivity of nanofiller can result in the remarkable increase of sensor sensitivity although the total initial resistance of sensor decreases remarkably in this case. These results imply that the key point to increase the sensor sensitivity is increase of either tunneling resistance or the ratio of the tunneling resistance to the total resistance, rather than the total resistance itself.

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