

# Thermal Performance Simulation of MWNT/NR composites Based on Levenberg-Marquard Algorithm

Z Z Yu<sup>1, a</sup>, J S Liu<sup>1, b</sup>

<sup>1</sup>College of Electromechanical Engineering, Qingdao University of Science & Technology, China 266061

E-mail: <sup>a</sup>yuzhenzhu@qust.edu.cn, <sup>b</sup>931669075@qq.com

**Abstract.** In this paper, Levenberg-Marquard algorithm was used to simulate thermal performance of aligned carbon nanotubes-filled rubber composite, and the effect of temperature, filling amount, MWNTs orientation and other factors on thermal performance were studied. The research results showed: MWNTs orientation can greatly improve the thermal conductivity of composite materials, the thermal performance improvement of overall orientation was higher than the local orientation. Volume fraction can affect thermal performance, thermal conductivity increased with the increase of volume fraction. Temperature had no significant effect on the thermal conductivity. The simulation results correlated well with experimental results, which showed that the simulation algorithm is effective and feasible.

## 1. Introduction

Natural rubber (NR) is a natural polymer with polyisoprene as a main component, with excellent resilience, insulation, impermeability and plasticity characteristics, widely used in transportation, construction, electronics, aerospace, oil chemical industry, agriculture, machinery, military, water conservancy and information industry, people's lives and other industries. But rubber is a poor conductor of heat, then a lot of heat generated under dynamic conditions cannot be derived in time, which will lead to high-temperature that damages rubber products performance and service life, so how to reinforce rubber thermal conductivity has become a hot topic[1-3]. Carbon nanotubes's (MWNTs) unique structure makes it have ultra-high strength and toughness, excellent electrical conductivity and thermal conductivity, which make MWNTs become the focus of scientific research in recent years[4]. He Yan[5] and the group members took it as a new enhanced thermally conductive filler to improve thermal properties of rubber, and then prepared a natural rubber composites; results showed that the thermal conductivity of rubber filled with MWNTs has been significantly improved compared with pure NR.

Based on the analysis on thermal properties of rubber filled with MWNTs, this paper has simulated the thermal conductivity of composite materials with a new type of back propagation algorithm and researched the influence of factors such as the ambient temperature, volume filling fraction, MWNTs-Orientatonon heat conduction, and wish to provide a reference for the study of the thermal properties of rubber composites filled with MWNTs.

## 2. The analysis on thermal conductivity of composite materials

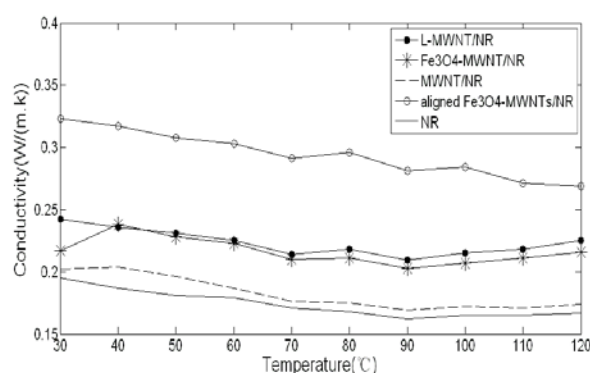
In this paper, MWNTs is filled in NR to improve the thermal conductivity of composite materials. This paper has studied the influence of the MWNTs' local orientation (local orientation means that



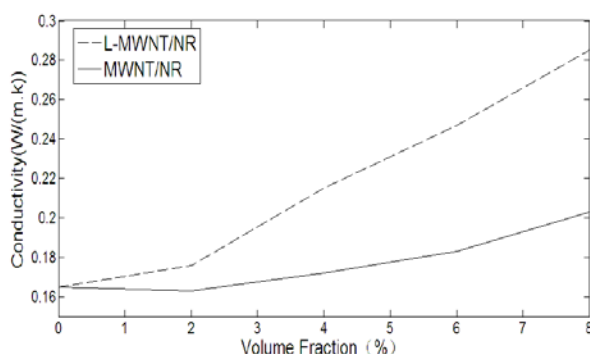
one dimension filler is arranged in orientation in micro area element, and scatters irregularly in global scope.), whole orientation and volume filling fraction on the thermal conductivity of NR composites in comparison with pure NR under the same conditions.

This group adopted[6] the method of solution blending to fill the rubber with MWNTs, local aligned carbon nanotube (L-MWNTs), Fe<sub>3</sub>O<sub>4</sub>-MWNTs magnetic nano composite particles respectively; and prepared MWNT/NR composites, L-MWNT/NR composites, Fe<sub>3</sub>O<sub>4</sub>-MWNT/NR composites, aligned Fe<sub>3</sub>O<sub>4</sub>-MWNT/NR composites by room temperature vulcanizing; finally obtained the thermal conductivity of composites with different volume filling fraction[7] by experiments.

Fig.1 shows the thermal conductivity of 4 kinds of composites filled with 4% volume fraction. The thermal conductivity of MWNT/NR composites, L-MWNT/NR composites, Fe<sub>3</sub>O<sub>4</sub>-MWNT/NR composites, aligned Fe<sub>3</sub>O<sub>4</sub>-MWNT/NR composites are all higher than that of natural rubber; and the conductivity of MWNT/NR composites is the lowest, thermal conductivity of the worst, the conductivity of aligned Fe<sub>3</sub>O<sub>4</sub>-MWNT/NR composites is the highest. Fig.2 shows the thermal conductivity of MWNT/NR composites, L-MWNT/NR composites at 100°C, which all increase with the increase of the filling fraction.



**Fig. 1** Thermal conductivity of MWNT filled NR compo-sites with 4% volume fraction



**Fig.2** Thermal conductivity of L-MWNT/NR composite at 100°C

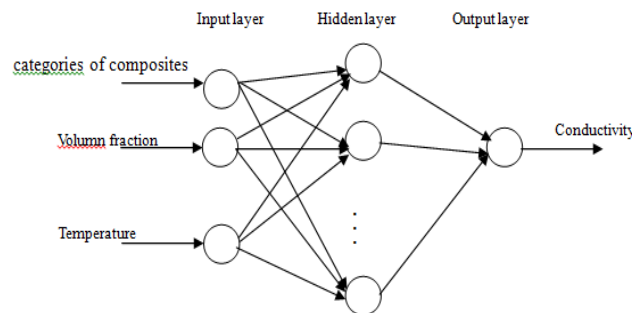
Experimental results show that 1) MWNTs can effectively improve the thermal properties of the composites, thermal conductivity of composites filled natural rubber with MWNT is greater than pure NR (see Fig.1, 2). Fe<sub>3</sub>O<sub>4</sub> particles have effectively improved thermal conductivity of the composites (see in Fig.1), the thermal conductivity curve of Fe<sub>3</sub>O<sub>4</sub>-MWNT/NR composites was significantly higher than MWNT/NR composites. 3) MWNTs orientation have effectively improved thermal conductivity of the composites (see Fig.1), the thermal conductivity of L-MWNT /NR composites is higher than that of non-directional composites. 4) The temperature had no significant effect (see Fig.1)

on the thermal properties of the composites. 5) The increase of filler fraction will improve the thermal conductivity of composites (see Fig.2), the relationship between the thermal conductivity and the filling volume fraction is non-linear.

### 3. Models and Methods

#### 3.1 Heat conduction model of MWNT/NR composites

Fig.3 shows the thermal model of MWNT/NR composites, the model is a three-layer forward network with three inputs and single output (a input layer, a hidden layer and a output layer), the inputs are categories of composites (see Table 1), volume filling fraction, ambient temperature, the output is thermal conductivity, the number of hidden layer nodes is 10.



**Fig.3** The thermal conductivity Model

**Table 1** Sample number

No.	composites
1#	Fe <sub>3</sub> O <sub>4</sub> -MWNT/NR
2#	MWNT/NR
3#	Aligned Fe <sub>3</sub> O <sub>4</sub> -MWNTs/NR
4#	L-MWNT/NR

The input nodes are chosen linear in this paper. The hidden layer of the node is [8]:

$$s_j = \sum_{i=1}^n w_{ji}^{(1)} x_i - \theta_j^{(1)}; \quad j = 1, 2, \quad (1)$$

In the formula (1),  $x_i$  is the  $i$ th input of the model,  $s_j$  is the input of the  $j$ th hidden node, and  $w_{ji}^{(1)}$  is the weights connecting the  $i$ th input node and the  $j$ th hidden node, and the  $\theta_j^{(1)}$  is the threshold of the  $j$ th hidden node. The output of the  $j$ th hidden node ( $O_j$ ) is:

$$o_j = f^{(1)}(s_j); \quad j = 1, 2, \quad (2)$$

In the formula (2),  $f^{(1)}(\cdot)$  is the activation function of the hidden nodes,  $f^{(1)}(x) = \frac{1}{1 + e^{-x}}$ . The output of the model is:

$$y = \sum_{j=1}^{10} w_{kj}^{(2)} o_j - \theta^{(2)}; \quad (3)$$

In the formula (3),  $\theta^{(2)}$  is the threshold of the output node, and  $w_{kj}^{(2)}$  is the weights connecting the  $j$ th hidden node and the output node.

#### 3.2 Levenberg-Marquard Algorithm

Levenberg-Marquard algorithm is a nonlinear optimization method, which combines the Gauss Newton method with gradient descent method. It is not sensitive to over parametric problem, and can effectively deal with nuisance parameter, so that the probability of the cost function falling into local minimum is reduced greatly. The above feature makes the LM algorithm widely used in the fields of model reconstruction, computer vision and so on. This paper used Levenberg-Marquardt algorithm to determine the parameters of thermal conductivity model. The weights of neural network are calculated as follows [9]:

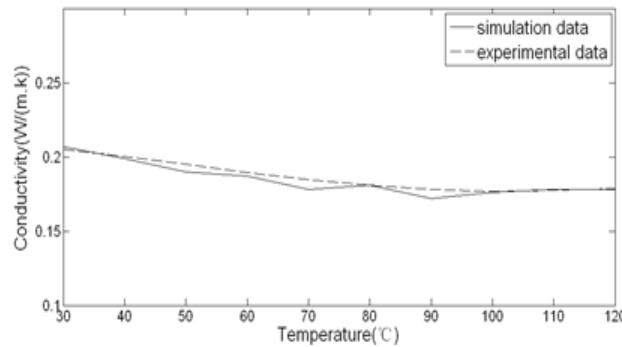
$$w(k+1) = w(k) - [J_k^T J_k]^{-1} J_k^T E_k \quad (4)$$

$$E_k = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_q \end{bmatrix} \quad (5)$$

In the formula (5),  $e_i = d_i - y_i$ ,  $d_i$  is the expected output of the model,  $q$  is the number of experimental data sets,  $k$  is the discrete time index,  $N$  is the number of weights.  $J$  is Jacobi matrix, defined as follows [9]:

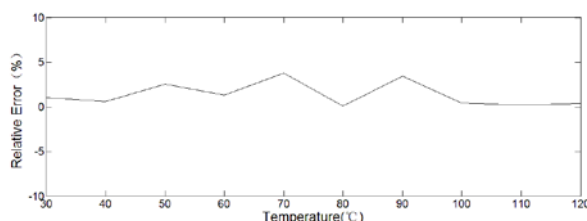
$$J = \begin{bmatrix} \frac{\partial e_1}{\partial w_1} & \frac{\partial e_1}{\partial w_2} & \dots & \frac{\partial e_1}{\partial w_N} \\ \frac{\partial e_2}{\partial w_1} & \frac{\partial e_2}{\partial w_2} & \dots & \frac{\partial e_2}{\partial w_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial e_q}{\partial w_1} & \frac{\partial e_q}{\partial w_2} & \dots & \frac{\partial e_q}{\partial w_N} \end{bmatrix} \quad (6)$$

### 3.3 Results and discussion



**Fig.4** Thermal conductivity of L-MWNT/NR composite with 2% volume fraction

This paper used Levenberg-Marquard algorithm to construct the thermal conductivity model of MWNT/NR composites, simulated the heat transfer performance of composites. Shown in Fig.4, Fig.5, the simulation results are in agreement with the experimental results, the error is small and the maximum relative error is 3.7%. The simulation results show that simulating the thermal conductivity of composites with Levenberg-Marquard algorithm is effective and feasible.



**Fig.5** Relative error

#### 4. Conclusion

Based on the analysis of the heat transfer performance of MWNT/NR composites, this paper used a new type of back-propagation algorithm to simulate the thermal performance of the composites, and investigated the influence of factors such as the ambient temperature, volume filling fraction, MWNTs-Orientation on heat conduction. The research showed:

1) MWNTs can effectively improve the thermal properties of the composites. 2)  $\text{Fe}_3\text{O}_4$  particles have effectively improved thermal properties of the composites. 3) MWNTs orientation can effectively improve thermal properties of the composites. 4) The temperature had no significant effect on the thermal properties of the composites. 5) The increase of filler fraction will improve the thermal properties of composites, the thermal conductivity increased with the increase of volume filling fraction, the relationship between the thermal conductivity and the filling volume fraction is non-linear. 6) The Levenberg-Marquard algorithm was used to simulate the thermal performance of composites, furthermore was used to research and analyse the influence of factors such as the ambient temperature, volume filling fraction, MWNTs-Orientation on heat conduction; the simulation results are accordant with the experimental results, that demonstrates the effectiveness of simulation algorithm and provides a new research approach for the study of thermal properties of rubber composites filled with MWNTs.

#### Acknowledgments

This work was supported by the National Natural Science Foundation of China under grant NO.51276091 and Collaborative Innovation Center of Green Tyres & Rubber NO.2014G7R0018.

#### References

- [1] Moniruzzaman M and Winey K I 2006 Polymer nanocomposites containing carbon nanotubes, *Macromolecules*, **39**, 16 5194-5205.
- [2] Shahil K M and Balandin A A 2012 Graphene-Multilayer Graphene Nanocomposites as Highly Efficient Thermal Interface Materials, *Nano Lett*, **12**, 2 861-867.
- [3] Sabyasachi G, Ajit K Roy, David P Anderson, et al 2008 Improved thermal conductivity for chemically functionalized exfoliated graphite /epoxy composites, *Carbon*, **46**, 5.806-817.
- [4] Tas D is, Tagmatarch N is, Bianco A, et al 2006 Chemistry of carbonnanotubes, *Chem. Rev.*, **106**, 31105-1136.
- [5] He Y, Feng J J and Ma L X 2013 Effect of Align-Carbon Nanotubes on the Properties of Nature Rubber Composite Materials *CJMR*, **27**, 5 495-500.
- [6] Anand K A, Sunil J T, Alex R and Joseph R 2010 Natural Rubber-Carbon Nanotube Composites through Latex Compounding, *International Journal of Polymeric Materials*, *Int. J. Polym. Mater.*, **59**, 1 33-34.
- [7] Feng J J 2013 Experimental Study on The Thermal Conductivity of NR Composite Filled with Orientational MWNTS, Qingdao University of Science & Technology, Qingdao.
- [8] Ge Z X and Shun Z Q 2007 Principles of Neural Network and MATLAB R2007 Realization, Electronics Industry, Beijing.
- [9] Fredric M, Ham and Ivica K 2007 Principles of Neurocomputing for Science and Engineering, China Machine Press, Beijing.