Thermal conductivity model for polymer/Boron Nitride nanocomposite considering air void content

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ABSTRACT

In this paper, we considered air void as the key parameter to improve thermal conductivity prediction model. Influences of air void on thermal conductivity of Polymer/BN nanocomposite was investigated by FEM based simulation. Thermal conductivity of composite was decreased with increase of air void content. In case of BN filler with 10 percent of volume fraction and thin layer air void model, thermal conductivity was decreased about 12 percent when we add air void with 1 percent of void content. Position and distribution of air void also influenced thermal conuductivity of nanocomposite. Thermal conductivity of nanocomposite decreased with an increase of contact surface area between air void and filler particle. For verifying these simulation results, we made Polymer/BN nanocomposite samples and analyzed their air void content by applying BET method and thermal conductivity by laser flash method. Influence of content and position of air void is not neglectable especially when the rate of formation of air void is high or air void formed between filler and matrix in the process of composite fabrication. If the parameters related to air void considered in thermal conductivity prediction model, prediciton model will be improved.

Keywords: nanocomposite, boron nitride, air void, thermal conductivity

1 INTRODUCTION

High thermal conductivity nanocomposites are widely used for cooling in many areas including electronic systems. Thermal property of polymer can be improved by adding appropriate fillers. Polymer/Boron Nitride (BN) nanocomposite is promising interfacial material for cooling of electronic systems due to high thermal conductivity, low thermal expansion, and high dielectric strength with simple process and relatively low cost [1-2]. It is important to determine minimum filler content where the thermal conductivity of nanocomposites starts to jump up when it practically uses in the industry. Various mathematical models predicting

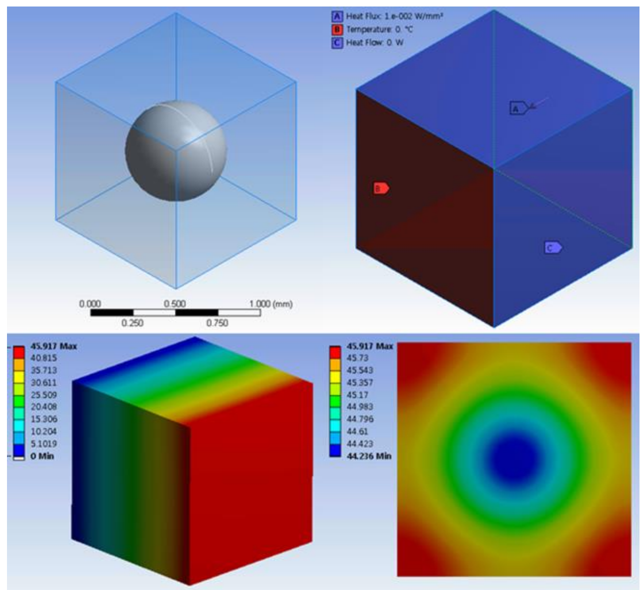
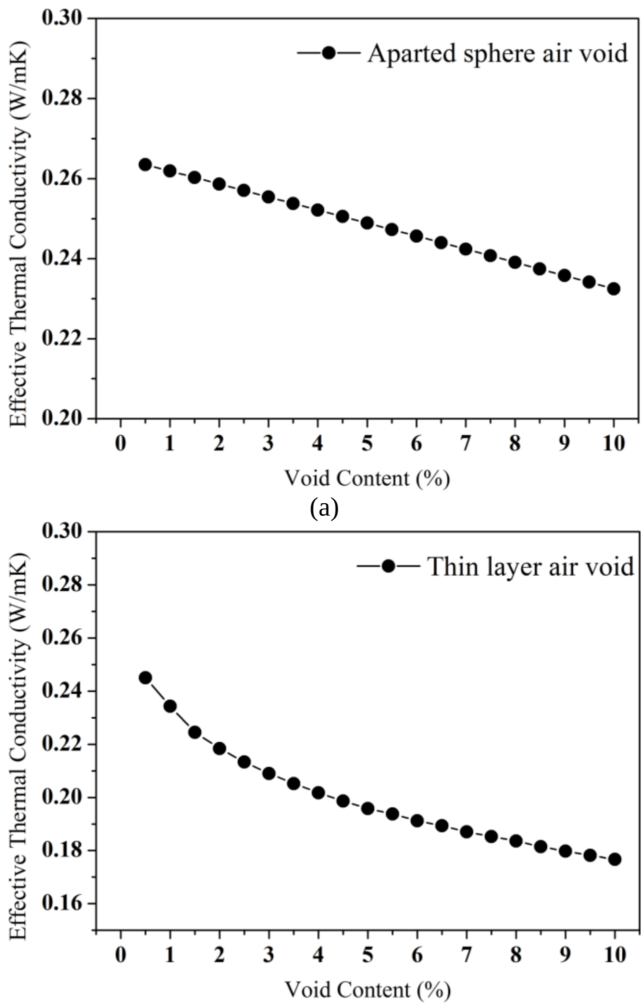


Figure 1: Geometry and boundary conditions of the basic thermal model.

thermal conductivity of nanocomposites have been proposed and investigated, but they have many limitations for exact prediction [3]. Most of models considered volume fraction of filler as a main parameter and many of other parameters are ignored and they assume that nanocomposite is mixture of only two materials, matrix and filler. Air void in composite materials also ignored, but nano/micro sized air voids are necessarily interfered in the nanocomposites during the mixing process. Thermal conductivity of air is very low and air void significantly influences on its thermal conductivity if air void exists between matrix and filler. BN nanocomposites are likely to hold more void due to the poor wettability, especially agglomeration of plate-shape BN is very porous [4]. Additional processes are performed to reduce the voids, but sometimes it is overlooked. Moreover, there was no quantitative measurement of void content of nanocomposites.

In this study, we investigated relationship between air void content and thermal conductivity of Polymer/BN nanocomposite and improve thermal condutivity prediction



(a)

(b)

Figure 2: Thermal conductivity of Polymer/BN composite with respect to air void content from simulation with (a) spherical air void apart from BN particle, (b) thin layer covering BN particle.

model. We considered air void as third material of nanocomposite and void content and position of void as key parameters. FEM based simulation was conducted for predicting influence of air void and we verified simulation result by real experiment.

2 EXPERIMENTAL

Thermal simulator (ANSYS Products v15) based on finite element method (FEM) was used in order to predict thermal conductivity of Polymer/BN nanocomposite and investigate void effect. We made model for very small part of nanocomposite because nanocomposite has too many particles to calculate whole system. Basic geometry of the model is comprised of a cubical epoxy resin and BN particles insdie the epoxy as shown in Fig. 1. BN particle is described as complete sphere. Thermal conductivity of BN and epoxy was 80W/mK, 0.2W/mK, respectively.

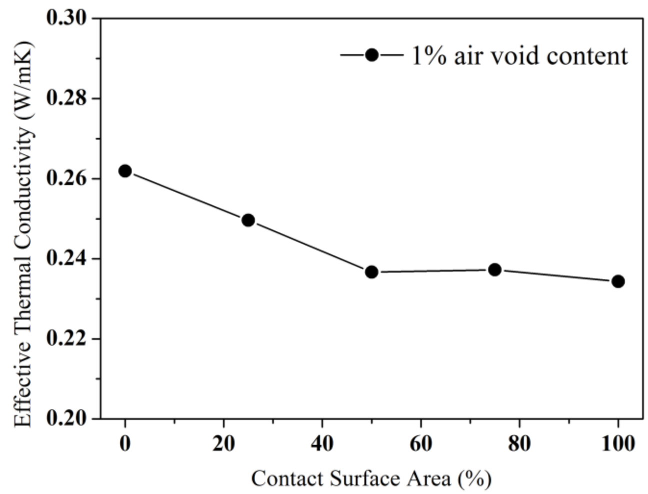


Figure 3: Thermal conductivity of Polymer/BN composite with respect to contact surface area between air void and BN filler particle.

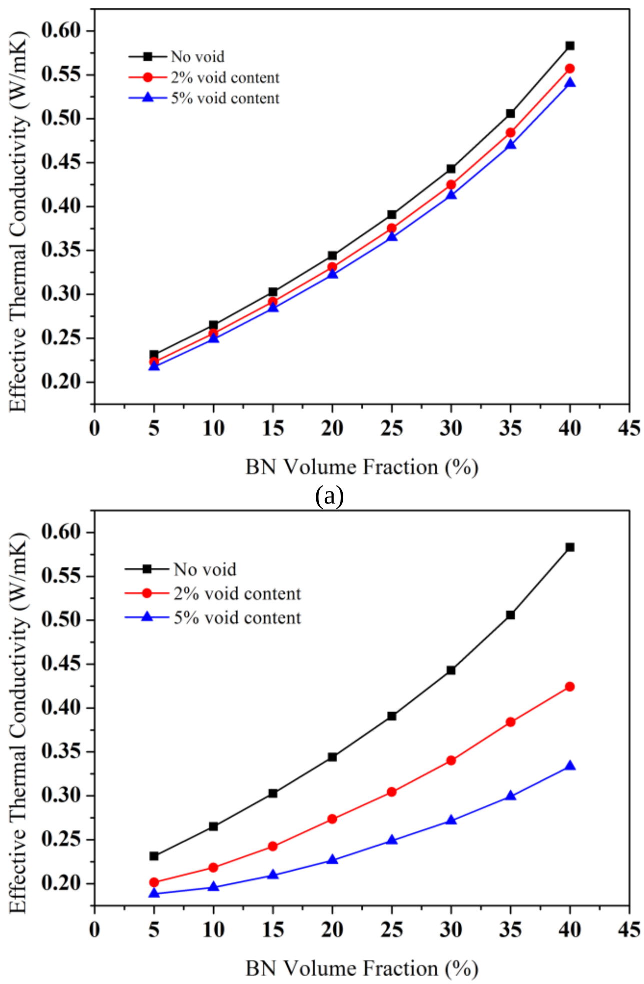
Heat flux (0.01W/mm^2) is applied at the one side of the epoxy (lower one of the z-axis) and temperature of the opposite side (higher side of the z-axis) is constant at 0℃. The other side is insulated (zero heat flow). Effective thermal conductivity (k_{eff}) is calculated from (1) under the assumption that the heat flows in one direction through a homogeneus material;

$$k_{eff} = \frac{Q}{\Delta T}\frac{L}{A} \tag{1}$$

Q is heat flux, ΔT is temperature difference between higher side and lower side of z-axis. Higher side is 0℃ and the temperature of lower side is averaged. A is cross-sectional area, L is thermal propagation length. We could control the BN or air void's volume fraction by changing the size of them with constant matrix size (side length of the cubical epoxy is 1 mm) in this model. We added air void in this model with different size and position.

Two kinds of void geometry and position were investigated; (i) spherical one apart from BN particle, (ii) thin layer covering the BN particle.

We made BN/Polymer nanocomposite samples with various BN volume fraction and void content to verify simulation result. Commercial hexagonal Boron Nitride(hBN) powders with size of 70nm, 500nm and 5000nm are prepared for filler material and two-component epoxy for matrix material. Commercial hexagonal-BN powder was dispersed by sonication within acetone and mixed with epoxy resin and hardener by using rotary paste mixer. The mixture was pressed by pellet press machine with different pressure and temperature in order to control the void content reproducibly. We analyzed void content by pore size distribution measured by Brunauer Emmett Teller (BET) method. Thermal conductivity was measured by laser flash method.



(a)

(b)

Figure 4: Thermal conductivity of Polymer/BN composite with respect to BN volume fraction from simulation with (a) spherical air void apart from BN particle, (b) thin layer covering BN particle.

3 RESULT AND DISCUSSION

To study relationship between air void and thermal conductivity, simulation was conducted using basic model with 10% BN volume fraction. Figure 2 shows the calculated thermal conductivity of Polymer/BN nanocomposite with spherical air void apart form BN particle and thiu layer air void covering BN the BN particle. Thermal conductivity of composite was decreased with the increase of air void content. In the thin layer type model, thermal conductivity was decreased about 12 percent when we add air void with 1 percent of void content. Addition of air void causes decrease of thermal conductivity because thermal conductivity of air is significantly low. Tendency of thermal conductivity is smillir in both model, however thin layer type air void causes more decrease of thermal conductivity. BN particle has high thermal conductivity and it is used filler material in nanocomposite. The air void between BN and polymer interrupt thermal conduction through BN particle that has higher thermal conductivity. Therefore, positon of air void also inflences thermal conductivity of Polymer/BN nanocomposite.

We conducted furthur simulation with respect to contact surface area between BN particle and air void to investigate relationship between postion of air void and thermal conductivity of Polymer/BN nanocomposite. Figure 3 shows thermal conductivity of Polymer/BN nanocomposite with respect to contact surface area between BN particle and air void in the same void content condition. Increase of contact surface area causes decrease of thermal conductivity of Polymer/BN nanocomposite as expected. However, we only considered contact surface area in this model and exceptional point was exist.

We conducted similar simulation with controlling volume fraction of BN particle for more general case. Thermal conductivity of Plymer/BN nanocomposite decreased with increase of air void content even if volume fraction was changed as shown in Figure 4. As a result of whole simulation, we predictied that air void content and position influence thermal conductivity of Polymer/BN nanocomposite. Thermal conductivity of nanocomosite decrease with increase of air void content and contact surface area between BN particle and air void.

To study real influence of air void and verify simulation result, we made Polymer/BN nanocomposite sampels with various BN volume fraction and air void content. Air void content was measured by applying Brunauer Emmett Teller method and thermal conductivity was measured by laser flash method. Organization of data is on progress and the experiment result data will be presented at the conference.

Thermal conductivity prediction model should be improved by including influence of air void. Because influence of air void is not neglectable especially when the rate of formation of air void is high or air void formed between filler and matrix in the process of composite fabrication. In the improved thermal conductivity predition model, air void content should be one of the major parameter and position of air void should be considered diffrently according to the type of nanocomposite. It is hard to predict whole distribution of void poistion in fabrication process. Therfore, it is better to calibrate prediction model using average distribution of air void according to type of nanocomposite.

4 CONCLUSION

In this research, we investigated influences of air void on thermal conductivity of nanocomposite by simulation. Thermal conductivity of composite was decreased with increase of air void content and contact surface area between air void and filler particle. Influence of content and position of air void is not neglectable especially when the rate of formation of air void is high or air void formed between filler and matrix in the process of composite fabrication. If the parameters related to air void considered in thermal conductivity prediction model, prediciton model will be improved.

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