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***Abstract*—With the trend of miniaturization and the increasing power density, the operating temperature of electronic devices keeps climbing, especially for wide band-gap semiconductors such as silicon carbide and gallium nitride. The high operating temperature up to 250℃ brings challenges to encapsulation materials since traditional encapsulation materials such as epoxy resins and silicone gels hardly bear temperatures above 200℃. Calcium aluminate cement (CAC) was proved to be a promising encapsulation material, which owns high thermal stability with its operating temperature of up to 300℃. Based on its satisfied thermal stability and low cost, the thermal conductivity of CAC was researched in this work with different ratios of 10-µm-sphere-Alumina (Al_2O_3) fillers at different temperatures, which formed µm-scale CAC-Al_2O_3 composites. In this work, we focused on the thermal conductivity of CAC-Al_2O_3 composites aiming for encapsulation applications in power electronics packaging. The thermal conductivities of µm-scale CAC-Al_2O_3 composites by the laser-flash method from room temperature to 350℃ were firstly measured. Results showed with an increasing content of fillers, the TC of CAC-Al_2O_3 will increase accordinglyIt also illustrated that calcium aluminate cement was a high thermal stable encapsulation material with thermal conductivity over epoxy resins. Then, the Finite Element Model (FEM) was established and calibrated by experimental data for thermal conductivity simulation. The FEM model accuracy reached 90%. Such models for new filler materials are effective to minimize material development by actual experiments and characterizations, for CAC composite with different fillers. It also provides an alternative method in predicting other physical properties of composites such as coefficient of thermal expansion, porosity, etc.**

Keywords*—*Encapsulation, Finite element modeling, Cement, Thermal conductivity, Electronic packaging.

I. INTRODUCTION

With the application of Silicon Carbide (SiC) and Gallium Nitride (GaN), the operating temperature of power modules is easily getting above 200°C. Sometimes the operating temperature reaches 250°C and higher. This high temperature brings a great challenge to encapsulation materials. The conventional encapsulation materials based on Si devices barely survive temperatures above 175°C [1, 2]. The most used encapsulation materials are silicone gel and epoxy resins. Both of them have severe reliability problems when the temperature is above 175°C, because of their lack of qualified thermal properties such as thermal conductivity and coefficient of thermal expansion. Therefore, there is an urgent need for a high-temperature stable encapsulation material. As Table I shows, cement possesses more excellent thermal properties than silicone gel and epoxy resin.

TABLE I. COMPARISON OF THERMAL PROPERTIES OF CEMENT, SILICONE GEL AND EPOXY RESIN

	Cement	Silicone gel	Epoxy resin
Highest operating temperature(°C)	>250	200	175
Thermal conductivity(W/mK)	>1	0.1-0.2	0.1-1
Coefficient of thermal expansion(ppm/K)	4-10	>300	30-60

Calcium aluminate cement (CAC) was proved to be a promising encapsulation material, which owns higher thermal stability than epoxy resins and silicone gels, with its operating temperature of up to 300°C [3]. Based on its excellent thermal stability, the next research target of CAC is to assess its thermal conductivity (TC). A high TC brings a high heat dissipation, which could lower the junction temperature of power modules. With a lowered junction temperature, the reliability and life of power modules will be greatly improved. It is not reported that the TC of CAC with μm-scale Alumina (Al_2O_3) fillers, to our best knowledge.

Hence, in this paper, the thermal conductivity of CAC was researched in this work with different ratios of 10-μm-sphere-Alumina (Al_2O_3) fillers at different temperatures by the laser-flash method. The results show that the highest TC is up to 1.547 W/mK with 80wt% of Al_2O_3 and porosity around 15%. Based on such results, the Finite Element Method (FEM) modeling was established for thermal conductivity calculation through COMSOL Multiphysics 5.5. CAC- Al_2O_3 composite with different filler ratios was modeled and calibrated. Based on such calibrated model, it is possible to forecast the properties of CAC composite with different fillers (e.g. silicon carbide),or different filler content, or under different porosity.

II. Experimental Investigations

A. Materials

Calcium aluminate cement was purchased from IMERYS Aluminates; 10-μm-Al_2O_3 powders were purchased from Qinghuangdao ENO High-tech Material Development Co., LTD; Additives were purchased from BASF SE.

B. Preparation of CAC-Al_20_3 composites

The preparation process of the CAC-Al_2O_3 composite is as follows. Firstly, calcium aluminate powders and alumina powders were intensively mixed with a stirrer for 5minutes. Secondly, after water treatment, the mixed paste was vacuum stirred to avoid air inducing with additives. Thirdly, the paste was cured at 60℃ for 3 hours, and then stewed for 48 hours at room temperature, with circular molding dimensions of 12.7 mm diameter with 2mm thickness, as Fig.1 shows. At last, the cured CAC-Al_2O_3 composite was demolded and then conducted heat preservation at 300℃ for 3 hours to fully eliminate the remaining water [4, 5].

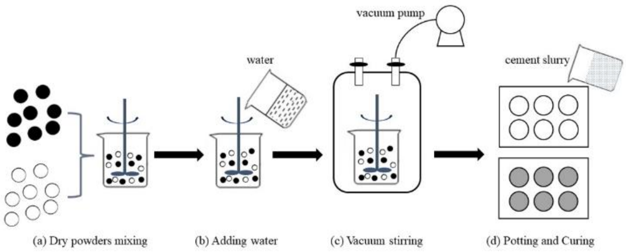

Fig.1 The process of smaple making

To minimize the data fluctuation, the sample surface was further polished and the finished samples were as shown in Fig.2. Thermal conductivity was then conducted through the laser-flash method through LFA 467, while the porosity of CAC-Al_2O_3 composite was tested by the Archimedes method。Each sample was measured three times and averaged.The specific tested TCs of CAC-Al_2O3 ranged with Al_2O_3 fillers from 10wt% to 80wt%.

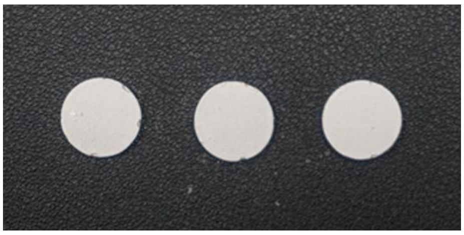

Fig.2 Samples for Laser-Flash method

C. FEM model

A two-ball model was established for different weight percentages of fillers, as Fig.3 shows. The representative volume element(RVE) consist of a square and two balls. One ball is in the core of sphere, and the other is equally divided to eight parts and set at eight vertices of square. The variation of the filler weight percentage is ranging from 10wt% to 80wt%, by changing the square side length from 25.34μm (10wt%) to 11.82 μm (80wt%). This distance reflects the density of CAC-Al_2O_3 composite, as the Fig.3 shows. In Fig.3(a) the distance between two balls is distinctly longer than in Fig.3(b), because the content of Al_2O_3 is only 10wt%. The spheres which represented for Al_2O_3 filler was set with a diameter of 10 μm based on the actual filler diameter applied and the rest part of the cube is cement. The highest weight percentage that two-ball model could reach is 84.45%.

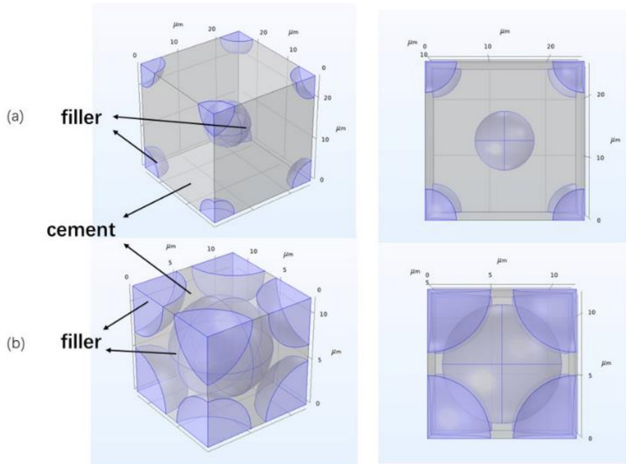

Fig.3 Schematic of two-ball model, model, (a) CAC-Al_2O_3 composite with 10wt% of Al_2O_3, (b) CAC-Al_2O_3 composite with 80wt% of Al_2O_3. The left is oblique drawing, and the right is side view.

After established the 3D models, the boundary conditions are as follow. One face of the cube was set to 293.15K, while the opposite face was 313.15K. The rest faces were adiabatic. Therefore, there was a temperature gradient in the RVE, and heat flux was obtained from the derived value in COMSOL. Porous media flow module of COMSOL 5.5 was chosen. The porosity was directly set in the cement base, that is the host material without specially establishing the holes, which simplified the establishment of RVE. The specific physical quantity of cement, air and Al_2O_3 filler are shown in the Table II.

Table II. Material properties applied in FEM model

	Thermal conductivity (W/mK)	Heat capacity (J/kgK)	Density (kg/m^3)
Cement	0.7	780	2800
Al_2O_3	30	3800	800
air	0.0025	1013	1.146

The interface resistance is also set at the surface of sphere to simulate the real situation. It should be cleared that interface resistance was only set at spherical surface, and the cut surface was considered continuous phase as the inner parts of ball, so there was no interface resistance set on cut surface.

$$q = -k\nabla T \quad (1)$$

q: heat flux(W/m^2)

k: thermal conductivity(W/mK)

∇T: temperature gradient(K/m)

TC was calculated through the heat flux and temperature gradient, which was directly gained from COSMOL, as the equation (1) showed.

D. TC of Laser-Flash method

The results of TC tested by the laser-flash method are shown in Fig.4. It was clear that with the increasing content of Al_2O_3, the TC increased correspondingly. This phenomenon was particularly evident when the content of Al_2O_3 increased to 80wt% from 60wt%. The increment of TC (60wt%-80wt%) enhanced drastically to 0.5 W/mK at temperature 25°C whereas increment of TC (20wt%-70wt%) was only around 0.2 W/mK. It was also observed that with temperature increasing, the TC of 80wt% CAC-Al_2O_3 composite decreased. It could be attributed to the interface resistance between Al_2O_3 filler and cement, which would increase with the increasing content of fillers. A higher interface resistance would hinder the heat transfer in CAC-Al_2O_3 composite, especially when temperature is arising. Hence, the TC of 80wt% CAC-Al_2O_3 composite kept decreasing since temperature above 100°C. This hypothesis is verified by the FEM model, which is calibrated by adjusting interface resistance.

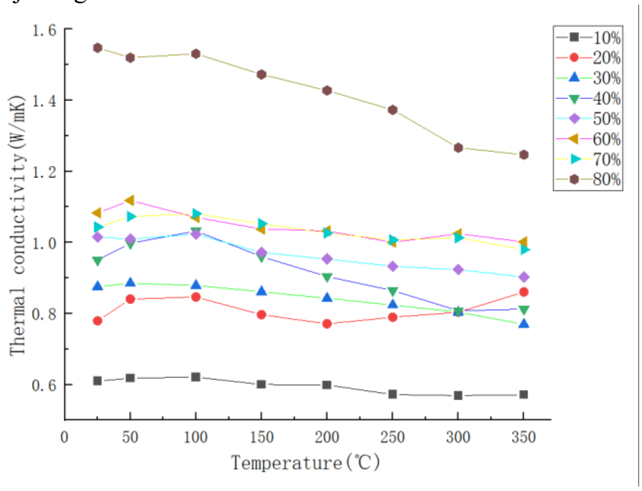

Fig.4 TC with different weight percentages at different temperatures tested by the Laser-Flash method

The highest TC is 1.547 W/mK with 80wt% of Al_2O_3 at 25°C. With such high doping content of Al_2O_3, the TC is still around 1.3 W/mK at temperatures as high as 350°C, at which epoxy resins and silicone gel could not survive at all. By contrast, the TC of epoxy resins and silicone gels is only around 0.1-0.2 W/mK [6]. Such high thermal stability and high TC make CAC-Al_2O_3 composite a promising substitute for encapsulation materials.

E. TC of FEM model

The results of simulated TC at 25°C are shown in Fig.5. The calibrated point is 80wt% with an interface resistance of 0.8×10^{-5} Km^2/W. According to the results, the points of 80wt%, and 60wt% matched with the experimental data. The points below 50wt% showed 10%-20% deviations from the experimental data, and the deviation values were all negative which meant the interface resistance set for high Al_2O_3 content composite (such as 80wt%) was too high for low Al_2O_3 content composite(10wt%-50wt%). In Fig.5 all the points were set with interface resistance of 0.8×10^{-5} Km^2/W. Such interface resistance was too large for CAC-Al_2O_3 composite with Al_2O_3 content under 50wt%. Therefore, the tested TCs from 20wt% up to 50wt% were higher than simulated TCs. The point of 70wt% did not match as other points, because the vacuum cup cracked by accident which induced air into CAC-Al_2O_3 composite and increased porosity during experiment. Unfortunately, due to the epidemic situation, the sample of 70wt% could not be retested. Therefore, the TC of 70wt% was approximately same as 60wt% and even a little bit lower than 60wt% at 25°C, which is clear shown in Fig.4 and Fig.5. However, the results suggested that interface resistance varied with different content of fillers. This is reasonable because with a higher content of Al_2O_3 fillers, the distance between two fillers will get closer that leading to a higher interface resistance. Generally, the interface resistance of the high content set is higher than the medium content set.

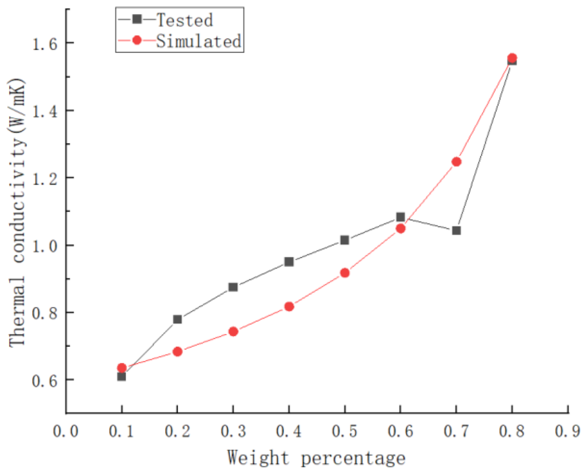

Fig.5 TC at 25°C with different weight percentages and interface resistance of 0.8×10^{-5} Km^2/W

It also needs to point out that the specific porosity of each sample varies and porosity is another dominant factor to TC, which could also explain why the tested and simulated TC of 10wt% was also matching with an obviously high interface resistance for 10wt%. Because the sample of 10wt% might have a higher porosity than 15%. Therefore, the exact interface resistance in every sample could not be tested or calculated precisely. But still, the interface resistance could be assessed in a confidence interval. As Fig.6 shows, after changing the interface resistance of 10wt% to 70wt%, the simulated TC was matching better and the deviations were below 10%. It proves that interface resistance varies with content of fillers and interface resistance gets larger with a higher content of fillers. The interface resistance applied in Fig.6 is concluded as equation (2). In this paper, the constant A for TC at 25°C was 10^{-5} Km^2/W. For example, the interface resistance of 10wt% was 0.1×10^{-5} Km^2/W and of 20wt% was 0.2×10^{-5} Km^2/W at 25°C.

$$R=AC \quad (2)$$

R: interface resistance (Km^2/W)

A: constant varies with different composite system which does not possess physical significance (Km^2/W)

C: content of fillers (%)

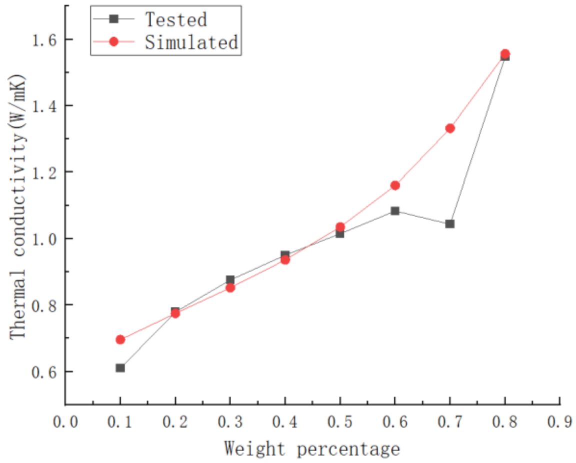

Fig.6 TC at 25°C with different weight percentages and different interface resistances

The law of interface resistance follows the distance between fillers which ranges from 1.82 μm (80wt%) to 15.34 μm (10wt%) according to the FEM model. This distance also stands for the amount of cement between fillers. It is clear that with distance getting closer the interface resistance is getting larger. Because all the samples were set with a porosity of 15% and when the content of cement is dropping the impact of holes gets stronger which is filled with air and hinder the heat transfer. This is why interface resistance is much bigger when content of fillers is at a high-doping level. As for the point of 10wt% and 60wt%, the deviation is probably because of a higher porosity.

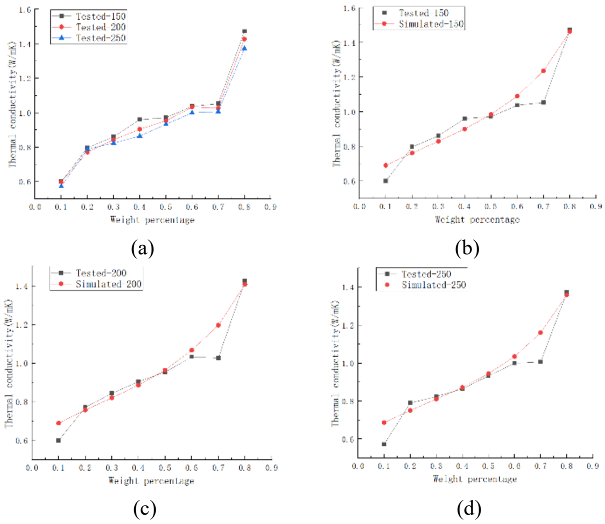

Fig.7 TC at 150°C, 200°C and 250°C with different weight percentages and different interface resistances(a) Tested results of TC at 150°C, 200°C and 250°C. (b) Tested and simulated results of TC at 150°C (c) Tested and simulated results of TC at 220°C. (d) Tested and simulated results of TC at 250°C

As the Fig.7(a) shows, TC decreased with a rising temperature. The decreasing level of TC was more obvious with a high content of Al_2O_3 fillers. This is because the real TC of Al_2O_3 fillers have a negative correlation with temperature and naturally with a higher content of Al_2O_3 fillers the TC decreased more at a higher temperature. At mean time, interface resistance also varies with temperature. Hence, TCs at 150°C, 200°C and 250°C were simulated based on equation (2) but with a different constant A. The calibrated point was still 80wt%. The constant A for 150°C, 200°C and 250°C was 1.25×10^{-5}, 1.375×10^{-5} and 1.5×10^{-5} Km^2/W, which meant the interface resistance of 150°C, 200°C and 250°C was 25%, 37.5% and 50% bigger than the interface resistance of 25°C, respectively. The tested TCs at 150°C, 200°C and 250°C were compared with simulated TCs as Fig.7(b)(c)(d) shows. These simulated results of TCs were matched with the ones at 25°C. The accuracy of such FEM model reached to 90%.

It needs to point out that interface resistance and thermal conductivity are correlated to temperatures. The TCs applied in this paper were assumed to be constants to simplify the calculation. Such FEM model greatly reduced actual experiments and provided rapid assessment to the TC of CAC composite. It is also possible to extend this FEM model to assess other physical quantities.

III. Conclusion

In this paper, CAC-Al_2O_3 composite was studied as encapsulation materials and the research was emphasized on its thermal conductivity. The CAC-Al_2O_3 composites containing 10-80wt% of Al_2O_3 were fabricated and TC of the CAC-Al_2O_3 composites were tested by the laser-flash method and simulated by the FEM models. The highest tested TC was 1.547 W/mK with 80wt% Al_2O_3. Based on such high TC, CAC-Al_2O_3 composite is promising as high-temperature encapsulation materials for power modules. The FEM module was established and proved to be effective in matching experimental data with interface resistance, with a simulation accuracy within 90%. An empirical formula was established to calculate interface resistance with different content of Al_2O_3 fillers. With such FEM modeling, the TC of composite with different fillers could be predicted, which saves time and minimize the experiments during developing CAC composite. Such modeling is also an alternative in predicting other properties such as coefficient of thermal expansion, porosity, etc.

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