Simulation, Prediction and Verification of the Thermal and Electrical Properties of Sintered Copper Joints with Random Pore Structure for Power Electronics Packaging

Liu, Wenting; Wang, Jianhao; Gao, Yue; Ji, Liangzheng; Zhang, Jing; Zhang, Guoqi; Liu, Pan

DOI
10.1109/ICEPT63120.2024.10668544

Publication date
2024

Document Version
Final published version

Published in
Proceedings of the 2024 25th International Conference on Electronic Packaging Technology, ICEPT 2024

Simulation, Prediction and Verification of the Thermal and Electrical Properties of Sintered Copper Joints with Random Pore Structure for Power Electronics Packaging

1st Wenting Liu
Academy for Engineering & Technology
Fudan University
Shanghai, China
22210860003@m.fudan.edu.cn

2nd Jianhao Wang
Heraeus Electronics
Heraeus Materials Technology Shanghai Ltd
Shanghai, China
jianhao.wang@heraeus.com

3rd Yue Gao
Heraeus Electronics
Heraeus Materials Technology Shanghai Ltd
Shanghai, China
yue.gao@heraeus.com

4th Liangzheng Ji
Academy for Engineering & Technology
Fudan University
Shanghai, China
21110860032@m.fudan.edu.cn

5th Jing Zhang
Heraeus Electronics
Heraeus Materials Technology Shanghai Ltd
Shanghai, China
j.zhang@heraeus.com

6th Guoqi Zhang
Department of Microelectronics
Delft University of Technology
Delft, the Netherlands
g.q.zhang@tudelft.nl

7th Pan Liu*
[1]*Academy for Engineering &Technology; Fudan University;*
Shanghai, China
[2]*Research Institute of Fudan University in Ningbo;* Ningbo, China
panliu@fudan.edu.cn

2024 25th International Conference on Electronic Packaging Technology (ICEPT) | 979-8-3503-5380-8/24/$31.00 ©2024 IEEE | DOI: 10.1109/ICEPT63120.2024.10668544

***Abstract*—Copper sintering has gained great attention as a die-attach technology for power electronics because of its potential cost effectiveness and high reliability under harsh working conditions. However, the mechanism of how the intrinsic pores within such sintered joints influence the thermal and electrical properties still needs further investigation. The evolution of pores within such sintered joints is difficult for in-situ observation during the sintering process and reliability tests, while the porosity level greatly affects the thermal and electrical properties. In this work, four two-dimensional (2D) models with various random pore structures were established based on the Quartet Structure Generation Set (QSGS) algorithm. Then, finite element method (FEM) simulations were conducted to simulate the heat and current conduction in the sintered materials. Subsequently, the distribution of temperature as well as the electric potential in the porous sintered materials were further discussed. Lastly, both the thermal and the electrical conductivities were calculated, followed by a concluded parabolic relationship of thermal and electrical conductivities with the porosity. These findings offer insights into optimizing and predicting copper sintered joint performance and accelerate the wide application of copper sintering.**

Keywords—copper sintering, porosity, thermal and electrical performance

I. Introduction

Sintering has emerged as a promising alternative die-attach technology for chip interconnection in power electronics, owing to its low processing temperature and excellent joint reliability [1]. Compared to traditional silver sintering, copper sintering offers potential cost efficiency, outstanding resistance to electromigration, and superior thermal and electrical performance [2]. However, copper sintering faces challenges such as elevated porosity, attributed to organic residues, oxide formation, and low diffusion rates, which considerably impact the overall reliability of the joints. Primarily, intrinsic air-filled pores within copper sintered joints lead to inefficient heat dissipation and increased electrical resistance. However, the intricate micro-mechanisms underlying such effects remain inadequately explored, thus require further investigation. Additionally, the porosity change, together with the evolution of pores, have been noticed for sintered joints during the sintering process and the following reliability tests. During sintering process, porosity is influenced by the volatilization of organic carriers as the temperature increases, as well as by the volume shrinkage of the sintered material itself [3]. While during reliability tests, pores inside the materials affect the mechanical and thermal stability, potentially leading to degradation and failure under operational stresses. However, accurate porosity levels during sintering and reliability tests are difficult to in-situ monitor for mechanism analysis. Thus, it is vital to investigate the impact of porosity, particularly with random pore structures, on the thermal and electrical performances of copper sintered joints through simulations.

In this work, four two-dimensional (2D) models with various porosity levels were firstly established, to simulate the random-shaped porous structures formed during the actual sintering process. After that, the influence of the porosity on the thermal and electrical properties of the joints was discussed and then quantified in mathematical equations. This study provides valuable insights into how porosity affect the thermal and electrical performance of the joints, hence further

advances the application of copper sintering in electronic packaging.

II. Model Construction and Sample Preparation

A. Simulation model construction

The Quartet Structure Generation Set (QSGS) algorithm has demonstrated high accuracy in generating structures of porous media, and widely adopted by researchers [4-6]. The algorithm introduced four key parameters to describe the generation and growth of pores: core distribution probability (C_d), directional growth probability (D_i), porosity (ε) or volume fraction (P_i), and interaction growth probability ($I_i^{n,m}$). The basic construction flow process of the QSGS algorithm was illustrated in Fig. 1(a) while the relative growth directions were shown in Fig. 1(b). Firstly, a certain number of the cores, which were based on the given distribution probability (C_d), were distributed randomly in the solid phase region as the initial nuclei of the pores. Secondly, the cores gradually grown up, as the growth of the pores in the sintering process due to particle volume shrinkage, along the directions in the given growth probability (D_i), until the porosity (ε) of material reached the set value. Lastly, the final 2D image of the porous material was constructed and output.

Based on the QSGS algorithm, four types of two-dimensional sintered porous structural images with porosities (ε) between 10% to 40% were generated. These images were then input into MATLAB and processed using a Kernel filter to smooth the edges, simulating the realistic structure of porous materials under various sintering conditions. Subsequently, the processed images were imported and converted into FEM models using the commercial software COMSOL. Assuming that only two phases existed in the sintered materials, the interaction growth probability was ignored during the construction process [7]. In this study, the core distribution probability (C_d) was set to 0.1, and the directional growth probabilities for D_{1-4} and D_{5-8} were both set to 0.2, indicating that the pores were assumed to exhibit isotropic growth.

B. Simulation parameters set up

Simulation parameters such as the input heat and current density as well as the boundary conditions are important. Fig. 2 presented the generated structural images of sintered joints (left) under different porosities levels and the corresponding meshed models (right) used for the thermal and electric performance simulations. To reflect realistic conditions, isolated solid phase clusters were removed from the images and not considered in the simulation models. In the simulations, the models were squares with dimensions of 30 μm by 30 μm. During the simulation process, the presence of pores at the upper and lower boundaries could cause significant variations in the thermal and electrical conditions. Therefore, two thin layers of copper, each with a thickness of 0.3 μm, were added to the upper and lower interfaces to standardize the input of heat and current density across all models. Then, the conventional grid was applied to mesh the models to accelerate and simplify the simulation process.

In all following simulations, the thermal conductivity and electrical conductivity of the copper material were set to 400 W/(m·K) and 5.9987E7 S/m, respectively. Considering the poor thermal and electrical conduction ability of such air-filled pores, both the left and right boundaries of the model, as well as the pore boundaries, were set to thermal insulation and electrical insulation conditions. In addition, we assume that the theoretical maximum thermal conductivity and electrical conductivity of porous copper has a negative linear correlation

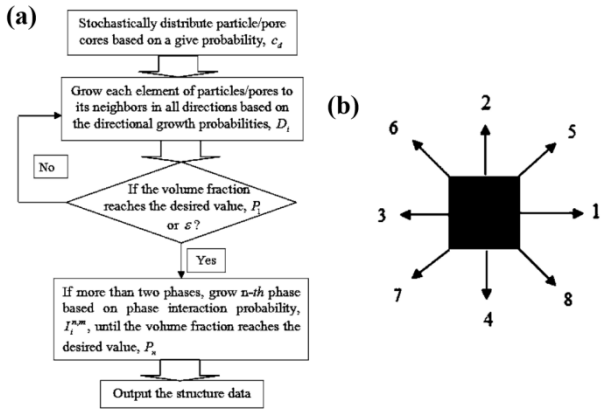

Fig. 1. (a) The flow chart of the porous structures construction; (b) the growth direction of the pore cores [7].

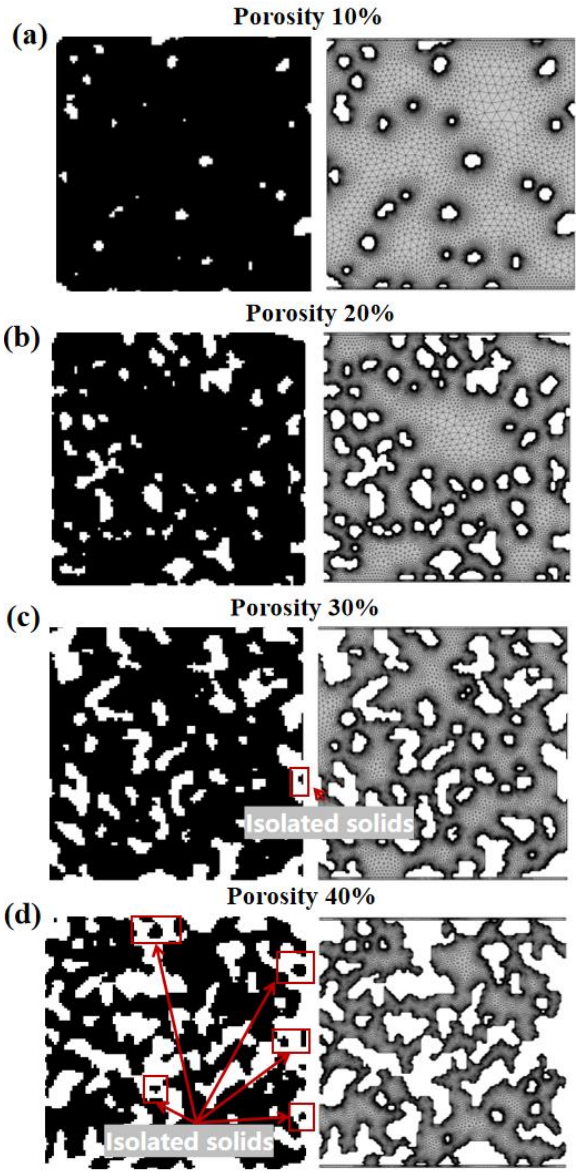

Fig. 2. The generated images (left) and the meshed simulation models (right) under different porosities levels

TABLE I. THE SINTERING PARAMETERS SET UP

Parameter	*Sample A*	*Sample B*
Sintering temperature (°C)	250	250
Sintering pressure (MPa)	10	20
Sintering time (min)	5	15

with porosity. That is, bulk copper is assumed to be 100% dense and has the highest thermal and electrical conductivity. While the porous material with a porosity of 20% was assumed to be 80% bulk copper. In the thermal simulations, heat flow (q) with a value of 1 W/mm² was applied to the top layer, and the temperature at the bottom layer was maintained at 298 K. In the electrical simulations, a current density (J) of 1 A/m² was applied to the top layer, with the bottom layer grounded. The thermal conductivity was derived using Fourier's law, and the electrical conductivity was determined based on the relationship between current density and electric field, as presented as (1) and (2).

$$q = -k\frac{dT}{dy} \tag{1}$$

$$J = \sigma E = \sigma\frac{dU}{dy} \tag{2}$$

Where the k is the thermal conductivity, dT is the temperature difference, $\sigma$is the electrical conductivity, dU is the electrical potential difference and dy is the heat/current transfer distance.

C. Sample preparation and characterization

The copper particles with an average diameter of 150 nm were applied (Ningbo Guangbo Nano New Materials) and then mixed with an alcohol-based system solvent (Shanghai Aladdin Biochemical Technology) to fabricate the copper paste. Then, two cylindrical samples were printed on the ceramic substrates. The diameter of the printing cylinder was 12.7 mm, and the printing height was 1 mm. After that, the samples were preheated at 150 °C for 30 minutes to evaporate the organic solvent. Then, samples were sintered in a sintering machine (Boschman SinterStar) by the thermocompression method under different sintering conditions in an N_2 atmosphere to obtain joints with various porosities. The detailed sintering parameters were listed in Table I. Lastly, the thermal conductivities of the cylinders were tested based on the laser flash method (NETZSCH LFA 467), and the electrical conductivities were measured through the four-probe test (NUOLEIXINDA RTS-8).

III. RESULTS AND DISCUSSIONS

A. Thermal performance simulation

To analyze the thermal performance of sintered joints, the temperature differences between the upper and lower interfaces of the simulation models need to be analyzed first. The average temperature differences between the upper and lower interfaces of sintered porous structures with different porosities were shown in Table II. The results indicated that as porosity gradually increased, both the average temperature and the average temperature difference between the interfaces also increased, suggesting that with higher porosity, there is a greater heat loss during the heat transfer process, which leads to a larger temperature difference between the upper and lower interfaces. Consequently, as the porosity of the sintered materials increase, the heat transfer capability of the porous material degrades, resulting in lower thermal conductivity. Not only the temperature difference, but it is worth further investigating the temperature distribution, temperature

TABLE II. AVERAGE TEMPERATURE AND TEMPERATURE DIFFERENCE OF POROUS SINTERING MODELS UNDER DIFFERENT POROSITY LEVELS

Porosity	*Avg. Temp. of the top layer (K)*	*Avg. Temp. of the bottom layer (K)*	*Avg. Temp. Difference (K)*
10 %	298.24	298.15	0.09
20 %	298.28	298.15	0.12
30 %	298.32	298.15	0.17
40 %	298.69	298.15	0.53

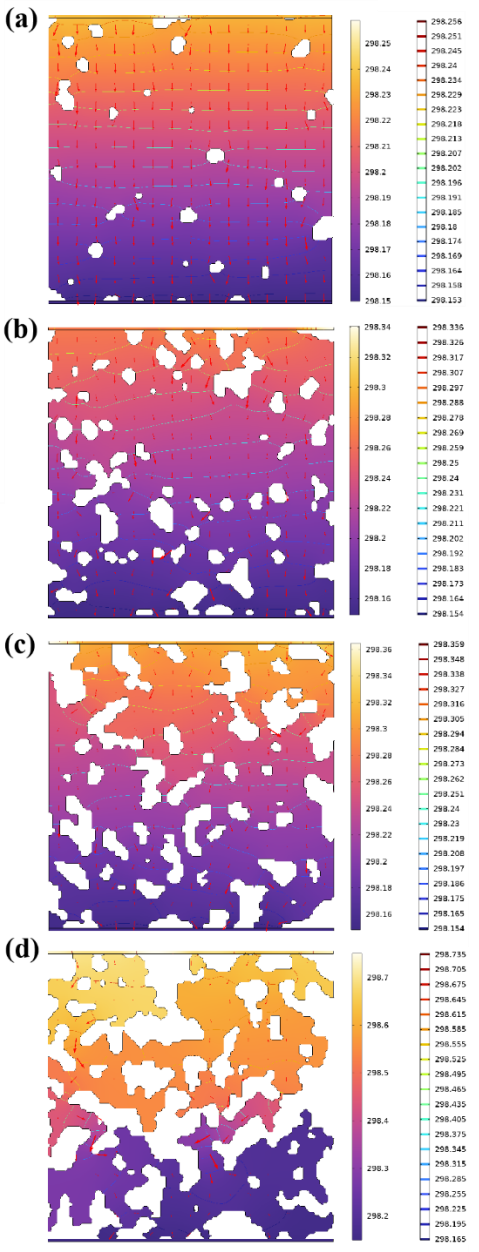

Fig. 3. The distributions of temperature, temperature contours, and heat flux of the simulation models under different porosities levels

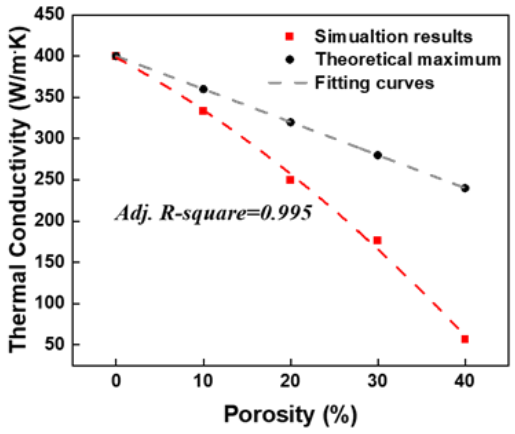

Fig. 4. Relationship between the porosity and thermal conductivity of sintered joints based on finite element simulation

contours, and heat flux flow of the simulation models, as displayed in Fig. 3. As porosity increased, the temperature contours became more irregular, indicating non-uniform heat transfer and suggesting that the sintered materials experienced uneven heating. Additionally, the direction of heat flux arrows revealed that heat flow concentrated mostly in the transport channels between closely spaced adjacent pores. Such a phenomenon was particularly pronounced especially when the porosity reached 40%. The close spacing between pores implied that the connections between solid phases were more fragile. Ultimately, heat gradually accumulated in these areas, leading to concentrated thermal stress, causing cracks and fractures to form around the pores, and finally failing the sintered joints.

To better clarify the relationship between the porosity of the sintered joint and its thermal properties from a simulation perspective, both the theoretical maximum and the simulated thermal conductivities of the materials under different porosity levels were calculated. Based on the assumption and (1), the theoretical maximum values were 360, 320, 280, and 240 W/m·K, respectively, while the simulated results were 333.3, 250.0, 176.5, and 56.6 W/m·K, respectively. Fig. 4 presented the relationship between the porosity of the joint and its thermal conductivities, including both the theoretical maximum values and the simulated results. The results showed a linear declining trend in the theoretical maximum values with increasing porosity, as assumed. In addition, the simulations revealed a negative parabolic correlation between joint porosity and simulated thermal conductivity.

According to the results, the pores in the sintered material significantly disturbed the heat transfer path and reduced the thermal conductivity of the material. The corresponding relationship between them was further quantified, as shown in (3).

$$k = -0.069 * \varepsilon^2 - 5.676 * \varepsilon + 398.2131 \qquad (3)$$

Where k is the simulated thermal conductivity and ε is the simulated material porosity. With the increase in porosity, the simulated thermal conductivity deviated greatly from the theoretical maximum thermal conductivity. When the porosity of the sintered materials reached 40%, the simulated thermal conductivity was 23.6% of the theoretical maximum value and was only 14.2% of the initial thermal conductivity, indicating that in materials with higher porosity, the pores have a more substantial effect on the heat transfer capacity of the sintered material due to the ununiform heat conduction path in the material.

TABLE III. AVERAGE ELECTRIC POTENTIAL AND POTENTIAL DIFFERENCE OF POROUS SINTERING MODELS UNDER DIFFERENT POROSITY LEVELS

Porosity	*Avg. Electric Potential of the top layer (V)*	*Avg. Electric Potential of the bottom layer (V)*	*Avg. Electric Potential difference (V)*
10 %	5.83E-13	4.96E-15	5.78E-13
20 %	8.38E-13	4.32E-15	8.34E-13
30 %	1.12E-12	6.77E-15	1.12E-12
40 %	3.57E-12	9.41E-15	3.56E-12

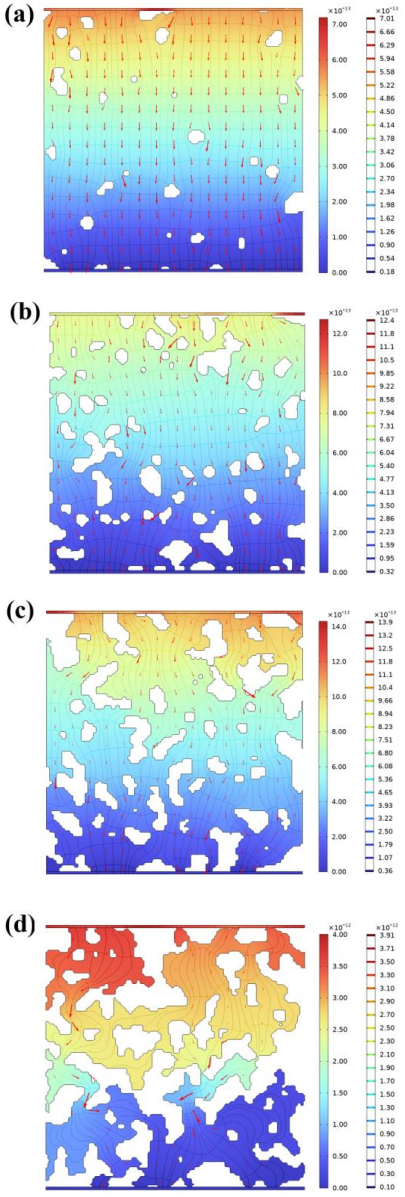

Fig. 5. The distributions of electric potential, electric potential contours, and current density of the simulation models under different porosities levels

B. Electrical performance simulation

Porosity level influences electrical performance of sintered joints. Firstly, the average electric potential differences were calculated, as shown in Table III. It

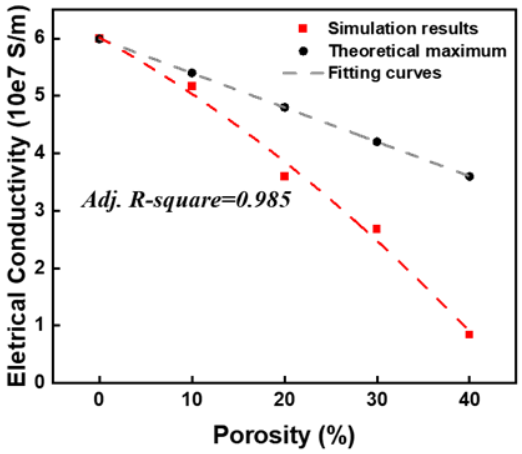

Fig. 6. Relationship between the porosity and electrical conductivity of sintered joints based on finite element simulation

presented the average electric potential difference at the upper and lower interfaces of sintered porous structures across different porosity levels. It was observed that both the average electric potential and the average electric potential difference at the upper and lower interfaces of the sintered material exhibited a general increasing trend. As a result of that, a heightened loss of electric energy was noticed during the current conduction process, which led to a successive degradation of the electric transfer capacity of the sintered material as well as a decrease in electrical conductivity.

Similar to thermal performance analysis, electrical performance simulations were further carried out for the electric potential distribution, electric potential contours, and current density flow direction (Fig. 5). As porosity increased, the contours of electric potential became more disordered, resulting in a non-uniform charge distribution inside the sintered material. Similar to the observations in thermal simulations, charge accumulated between pores with narrow spacing. The current flowing through these "narrow" channels generated a significant amount of heat, particularly for sintering structures with high porosity. Such heat-generating effect of electric transfer may accelerate the dramatic decline in material properties due to thermal failure.

Similarly, based on the assumption and (2), the theoretical maximum electrical conductivities of the materials under different porosity levels were calculated as 5.40E7, 4.79E7, 4.20E7, and 3.60E7 S/m, respectively while the simulated values were 5.17E7, 3.60E7, 2.68E7, and 0.84E7 S/m, respectively. Fig. 6 presented the relationship between the porosity of the joint and its electrical conductivities, including both the theoretical maximum values and the simulated results. The results showed a linear declining trend in the theoretical maximum values with increasing porosity, as assumed. Differently, the simulations revealed a negative parabolic correlation between joint porosity and simulated electrical conductivity.

According to the results, it presented that the pores in the sintered material significantly disrupted the current transfer process within the material, leading to a reduction in conductivity. This relationship was quantified in a mathematical equation, as presented in (4).

$$\sigma = (9.925e-4) * \varepsilon^2 + 0.088 * \varepsilon + 6.015 \qquad (4)$$

Where σ is the simulated conductivity of the material and ε

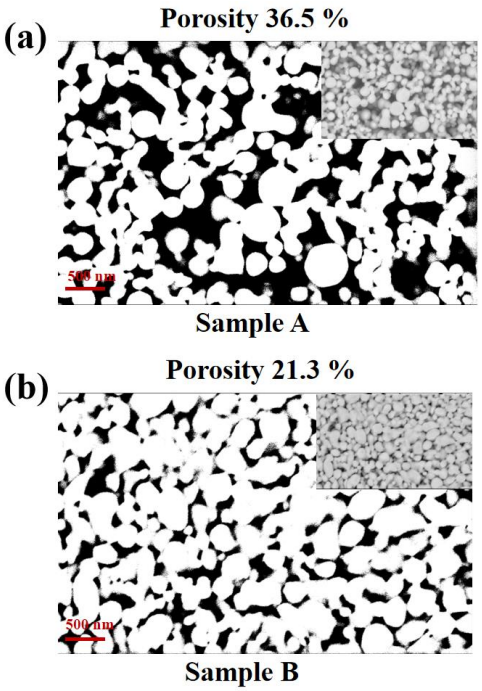

Fig. 7. The binary cross-sectional images and original images of the cylindrical samples under different porosities levels

TABLE IV. THE COMPARISON BETWEEN THE TEST RESULTS AND THE SIMULATED RESULTS OF THE THERMAL AND ELECTRICAL CONDUCTIVITIES

Performance	*Sample A*	*Sample B*
Thermal conductivity W/m·K	31.56	85.61
Simulated thermal conductivity W/m·K	99.11	246.00
Electrical conductivity 10E7 S/m	0.68	0.89
Simulated electrical conductivity 10E7 S/m	4.12	4.59

is the simulated porosity of the material. Similar to the thermal properties, the simulated electrical conductivity deviated from the theoretical maximum electrical conductivity as porosity increases. When the porosity of materials reached 40%, the electrical conductivity of the material was 23.3% of the theoretical maximum value and was only 14.0% of the initial electrical conductivity, suggesting that in materials with higher porosity, the pores have a more significant effect on the current transfer capacity of the sintered material.

C. Experimental verification

Two cylindrical samples with different porosity levels were fabricated under different sintering processes and the binary cross-sectional pictures as well as the original images were presented in Fig. 7. Meanwhile, the test thermal conductivities and electrical conductivities were shown in Table IV in comparison with the simulated results derived from (3) and (4), respectively.

Sample A exhibited the higher porosity since it was sintered with lower pressure as well as lower time, resulting in lower thermal and electrical conductivities. Relatively, Sample B had the lower porosity and higher thermal as well as electrical conductivities since the higher sintering pressure

and sintering time were applied to accelerate the densification of the sintered copper. More sintering necks formed during this process. However, compared to the test results, the simulation values were much higher. This discrepancy can be attributed to the following reasons: On one hand, the organic solvent may not evaporate thoroughly during the sintering process, and their residues dramatically influence the related test results due to their characteristics of thermal and electrical isolation. On the other hand, the formation of potential copper oxides also greatly decreases the thermal and electrical performance of the joints.

In this work, the influence of the different porosity levels of the sintered joints on thermal and electrical performances were discussed through the FEM simulations. The relationship between the porosity and the thermal as well as electrical conductivities was quantified in mathematical equations and then verified through practical experiments. However, the effect of the random pore structure under the same porosity is ignored in these ideal simulations. Furthermore, additional construction of the three-dimensional (3D) models is required to more accurately recreate the pore structures formed during the actual sintering process.

IV. Conclusions

In this study, 2D random pore structure models of sintered copper joints with porosities of 10%- 40% were firstly constructed using the Quartet Structure Generation Set (QSGS) algorithm. Subsequently, corresponding Finite Element Method (FEM) simulations were conducted to investigate the effects of porosity on the thermal and electrical performances of the sintered joints. The relationship between porosity and thermal/electrical conductivities of the sintered joints was further elucidated and analyzed. After that, the experiments were conducted to verify the quantified mathematical relationship. Here are some conclusions: Firstly, the existence of pores in sintered joints dramatically disrupted both heat transfer and electrical conduction pathways. Higher porosity levels tended to disorder these pathways, leading to irregular heat transfer and electrical conduction routes, and resulting in an uneven distribution of temperature and electric potential within the material. Secondly, the accumulation of heat and current around pores with minor spacing led to the elevated temperatures and electric potentials in those regions, accelerating the formation of cracks and fracture due to the concentrated thermal stress, thereby increasing the risk of joint failure. Thirdly, a parabolic negative correlation was revealed between porosity and the thermal/electrical conductivity of sintered joints. As porosity increases, this negative effect became more pronounced.

In summary, this work investigated the influence of porosity on the thermal and electrical properties of sintered copper joints, using a combination of the QSGS algorithm and FEM simulations, and provided valuable insights for optimizing sintered copper joints in power electronics packaging. With such a method, it also provides a future possibility to investigate the random pores with different parameters considering the size, shape, and distribution.

Acknowledgment

Funding for this research was provided by Shanghai SiC Power Devices Engineering & Technology Research Center (19DZ2253400) and the Natural Science Foundation of China (62304051). Many thanks to the Chat Generative Pre-Trained Transformer (ChatGPT, OpenAI) for linguistic assistance and Heraeus Materials Technology Shanghai Ltd. for support with characterization.

References

[1] F. Roccaforte, P. Fiorenza, G. Greco, R.L. Nigro, F. Giannazzo and F. Iucolano et al., "Emerging trends in wide band gap semiconductors (SiC and GaN) technology for power devices," Microelectronic Engineering, 2018, vol. 187-188, pp. 66-77.

[2] M. Wang, Y. Shan, Y. Mei, X. Li, and G. Lu, "Sintered-copper Die-attach: Processing, Properties, and Reliability," in CIPS 2020; 11th International Conference on Integrated Power Electronics Systems, 2020, pp. 1-6.

[3] S. Chen and H. Zhang, "Silver Sintering and Soldering: Bonding Process and Comparison," in Die-Attach Materials for High Temperature Applications in Microelectronics Packaging: Materials, Processes, Equipment, and Reliability, K. S. Siow Ed. Cham: Springer International Publishing, 2019, pp. 1-33.

[4] R. Li, Z. Wang, H. Dong, M. Yang, X. Sun and Q. Zong et al., "Lattice Boltzmann modeling of the effective thermal conductivity in plant fiber porous media generated by Quartet Structure Generation Set," Materials & Design, 2023, vol. 234, p. 112303.

[5] H. Shi, C. Y. Zhao, and B. X. Wang, "Modeling the thermal radiation properties of thermal barrier coatings based on a random generation algorithm," Ceramics International, 2016, vol. 42, no. 8, pp. 9752-9761.

[6] H. Zhang, H. Yu, S. Meng, M. Huang, M. Micheal and J. Su et al., "Fast and accurate reconstruction of large-scale 3D porous media using deep learning," Journal of Petroleum Science and Engineering, 2022, vol. 217, p. 110937.

[7] M. Wang, J. Wang, N. Pan, and S. Chen, "Mesoscopic predictions of the effective thermal conductivity for microscale random porous media," Physical Review E Statistical Nonlinear & Soft Matter Physics, 2007, vol. 75, no. 3, p. 03670.