

Thermal Management of TSV Array in 3D Integrated Circuits Based on the Super-Element Method

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Abstract: As Moore's Law approaches its physical limits, three-dimensional integrated circuits (3D ICs) utilizing Through-Silicon Vias (TSVs) are gradually replacing traditional two-dimensional integrated circuits (2D ICs). However, the highly integrated circuits also introduce more significant thermal issues. In this paper, an optimization method for the positions of multiple heat sources in the TSV array is proposed to minimize the temperature and temperature gradient within the model. This study employs super-element methods for thermal simulations, leverages the superposition principle to reduce the computational cost, and utilizes Simulated Annealing (SA) for position optimization. Experimental results show that the time required for the super-element method to compute the simulation model is approximately 26.4% of that required by FEM. Furthermore, after optimization, the maximum temperature rise, average temperature rise, and temperature gradient of the TSV array are reduced by 4.58%, 0.64%, and 3.78%, respectively, significantly mitigating the thermal effects on the circuit.

Keywords: Thermal management, TSV, Super-Element, FEM

1. Introduction

With the continuous development of integrated circuits, Moore's Law is gradually approaching its physical limits. The bottlenecks of traditional 2D ICs are becoming increasingly apparent, making it difficult to meet the demands of modern electronic devices for high performance and miniaturization. In this context, 3D IC, which can vertically stack multiple chip units, achieve higher integration density.

In 3D IC technology, TSVs play a crucial role. TSVs enable signal transmission and thermal conduction between chips by vertically drilling holes in the silicon wafer and filling them with conductive materials [1]. However, due to the vertical stacking structure of 3D ICs, which significantly increases power density, the temperature within the chips rises substantially. Therefore, the thermal issues within the chips urgently need to be addressed.

As 3D IC technology has developed, the application scale of TSVs has gradually expanded. In practical designs, to meet the demands for high integration, TSVs are typically deployed in large arrays within chips. However, the scale of TSVs significantly increases the computational complexity of thermal simulations, making it difficult for traditional simulation methods to balance precision and efficiency when facing such large-scale computations.

In recent years, research on the thermal behavior of TSVs has mainly focused on the following aspects: 1) Establishing thermal simulation models to analyze the thermal conduction characteristics of TSVs under different materials [2], [3], geometric structures [4], and array configurations [5], [6]; 2) Studying the thermal stress issues of TSVs and their impact on system reliability [7]–[9]; and 3) Optimizing the thermal performance of TSV structures under different constraints [10]. The issue addressed in this paper falls under the third category, specifically optimizing the positions of heat sources to reduce the temperature within the TSV array.

Regardless of the research topic, it is essential to first select an appropriate thermal simulation method. Among these, the equivalent thermal network method [2], [3], [10], [11] is a simple and efficient simulation approach, but it often fails to meet high-precision simulation requirements. In recent years, with the rapid development of artificial intelligence technology, machine learning based thermal simulation methods, such as Physics-Informed Neural Networks (PINN) [12], [13], have gradually gained popularity. However, these methods rely on high-quality training data and incur significant training costs. In contrast, numerical methods (such as the finite volume method [14] and finite element method [8], [9]) can accurately simulate thermal behavior but have high computational complexity, which significantly limits their application in large-scale systems [15].

To optimize the placement of heat sources, this paper develops a high-precision thermal simulation model for TSVs using the super-element method. Next, the principle of superposition is applied to simplify the algorithm for simulations with multiple heat sources. Finally, we proposed an optimization method for heat source positions based on heuristic algorithms, aimed at enhancing the thermal dissipation performance of TSVs and improving the overall thermal reliability of 3D ICs. This research provides valuable insights into thermal management technologies for 3D ICs.

2. Model of TSV Array

3D IC model: The thermal model used in this paper is a simplified version of the 3D IC interconnect model, as shown in Fig. 1. The main body of the model consists of multiple layers of dies, with TSV arrays evenly distributed across each die. Micro bumps connect adjacent TSV layers, with the spaces between them filled with underfill material. The uppermost die lacks TSVs and is equipped with a heat sink. At the bottom, the package substrate is placed beneath the lowest layer of micro bumps.

TSV model: The TSV model is shown in Fig. 2. Its primary component is a cylindrical copper column, surrounded by a thin oxide coating that covers both the bottom and top of the die. The rest of the die is filled with silicon.

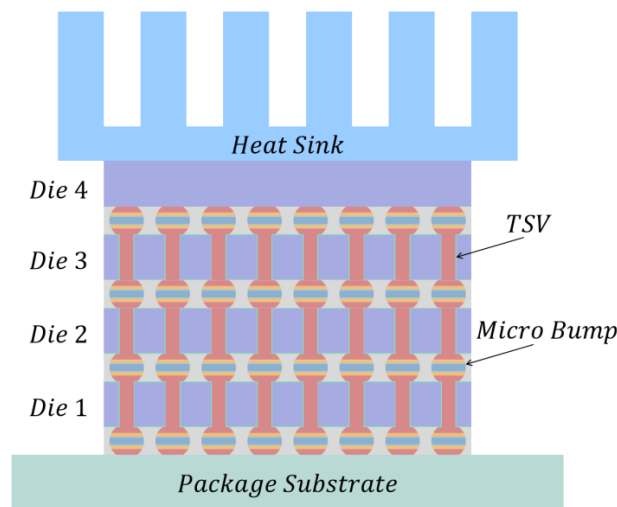


Figure 1: Illustration of the 3D IC Model

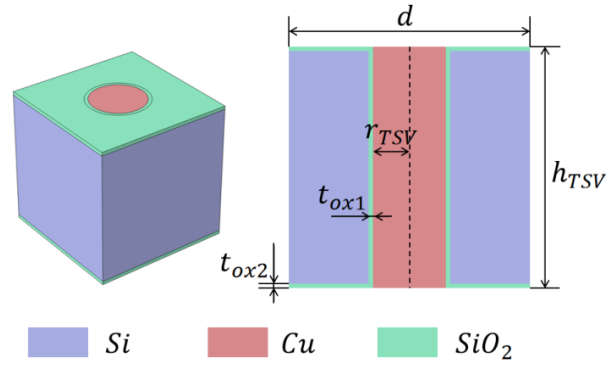


Figure 2: Illustration of the TSV Model

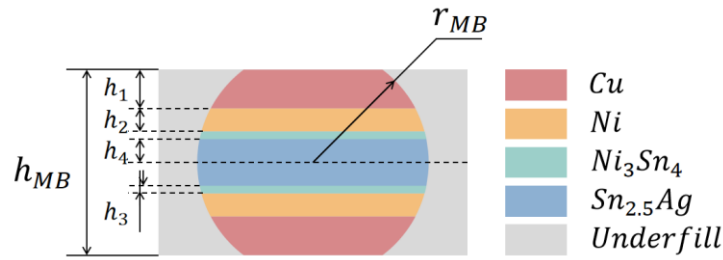


Figure 3: Illustration of the Micro Bump Model

Micro bump model: The micro bump model is shown in Fig. 3. The primary component can be simplified as a multi-layer structure in the shape of a spherical cap. The rest part is filled with underfill material.

3. Simulation Method

The objective of this paper is to optimize the positions of multiple heat sources in the TSV arrays to minimize the temperature and temperature gradient in the model. To accomplish this goal, three steps need to be completed:

- 1) Due to the larger scale of the TSV arrays, it is necessary to use an algorithm with low computational cost for thermal simulation.
- 2) Based on the thermal simulation algorithm in Step 1, proposed an algorithm that can quickly obtain the temperature data according to the positions of multiple heat sources.
- 3) Compute the objective function using the data and optimize the positions based on it.

3.1. Thermal Simulation Using the Super-Element Method

Given the periodicity of the TSV arrays, the super-element method is used in Step 1.

The super-element method is based on the finite element method, which is a numerical analysis technique used to solve approximate solutions to physics problems. It is particularly suitable for dealing with structures and systems with complex geometry, material properties and boundary conditions. In this article, the Fourier equation with boundary heat source conditions is employed:

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

$$n \cdot (k\nabla T) = Q_s \quad (2)$$

where k is the thermal conductivity, and Q_v and Q_s are the body heat source and boundary heat sources respectively.

In the finite element method calculation process, solving the linear equations is the most computationally intensive step. For the direct method, the time complexity of solving an n -order system of linear equations is $O(n^3)$. This method is extremely inefficient for large-scale TSV arrays. Especially when the goal is to optimize the positions of heat sources, calculating the temperature under a large number of different conditions is necessary, which imposes higher requirements on the algorithm's time complexity.

Therefore, given the periodicity of the TSV array, this paper employs the super-element method to reduce the time complexity. The super-element is a structure composed of multiple elements that roughly divides the overall geometry. Since each super-element can be regarded as an independent geometry, the temperature of the nodes in the super-element satisfies the following linear equations:

$$Kx = b \quad (3)$$

In particular, when the geometric structure of each super-element is identical, its mesh division can also be exactly the same. Therefore, the formula (3) for each super-element is the same, which further reduces the computational cost.

Since there are overlapping nodes (boundary nodes) between super-elements and internal nodes have no direct influence on other super-elements, it is natural to separate internal nodes from boundary nodes, i.e.

$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad (4)$$

where x_1 and x_2 represent the temperature of boundary and internal nodes, respectively, and

$$(K_{11} - K_{12}K_{22}^{-1}K_{21})x_1 = b_1 - K_{12}K_{22}^{-1}b_2 \quad (5)$$

$$x_2 = K_{22}^{-1}(b_2 - K_{21}x_1) \quad (6)$$

By combining equation (5) for all super-element boundary nodes into a global equation, the temperature of all boundary nodes can be solved. Then the temperature of the internal nodes of each super-element can be obtained by (6).

Assume that there are n elements and m super-elements, with each super-element containing n_{bnd} boundary nodes and n_{int} internal nodes. When the number of super-elements is sufficiently large, it can be assumed that each boundary node exists in two super-elements. Therefore,

$$\frac{mn_{bnd}}{2} + mn_{int} \approx n \quad (7)$$

In the super-element method, the computationally heavy steps consist of three parts: calculating the matrix in (5), solving the global equation, and calculating the temperature of internal nodes of each super-element through (6). Then the time complexity is about

$$O\left(\left(\frac{mn_{bnd}}{2}\right)^3 + mn_{int}^3\right) \quad (8)$$

which shows significant reduction in computational cost since $n_{int} > n_{bnd}$ in most cases.

This paper uses a rectangular-arranged TSV array as an example. The super-element is divided as shown in Fig. 4, with each super-element containing a TSV and a micro bump. The number of super-elements in three directions are m_x , m_y , and m_z , respectively, which satisfies $m = m_x \times m_y \times m_z$.

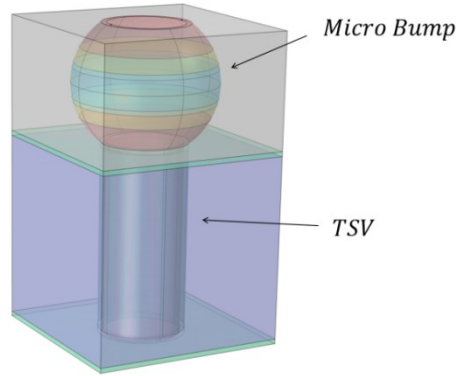


Figure 4: Illustration of Super-Element

3.2. Multi-Heat Source Simulation Based on Superposition Principle

The heat source in an actual circuit is often complex and large in scale. Since the movement of the heat source over a small distance has little effect on the temperature, this paper simplifies the size of the heat source to $a \times b$, where a and b are integers. An example of heat source is shown in Fig. 5. Define $\mathbf{S} = \{s_1, s_2, \dots, s_k\}$ as the set of all heat sources. For all $i \in \{1, 2, \dots, k\}$, the size of s_i is $a_i \times b_i$ and its power is Q_i .

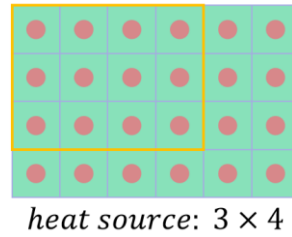


Figure 5: Example of Heat Source

Although the super-element method can significantly reduce the computational cost of the simulation, thermal simulation on a large number of models with different $\mathbf{S}$ is required in the process of optimizing the heat source positions. It is obviously unrealistic to perform the super-element method for each simulation. Therefore, this paper applies a multiple heat source simulation algorithm based on the superposition principle to further reduce the computational cost.

The thermal superposition theorem is an important concept in heat conduction theory, primarily used for the linear heat conduction problems. It states that for multiple heat sources in a linear system, the effects of each heat source can be superimposed to obtain the overall response of the system.

The steps of the heat simulation algorithm based on the superposition principle are as follows:

- 1) Select an arbitrary super-element, apply a heat source with arbitrary power to the super-element, and use the super-element method to calculate the temperatures of all nodes in the model. Then, record the temperature data. Perform the same operation for each super-element.
- 2) For any given $\mathbf{S}$, select the corresponding data from the stored temperature data, and obtain the temperatures of all nodes in the model using the principle of superposition.
- 3) Calculate the objective function based on the node temperatures.

3.3. Optimization of Heat Source Positions

Before optimizing the heat source positions, a suitable objective function needs to be established. This paper selects three commonly used objective functions: maximum temperature, average temperature, and maximum temperature gradient. The calculation methods for the three objective functions are as follows:

Maximum temperature: Select the maximum temperature directly among the nodes.

Average temperature: The average temperature cannot simply be obtained by averaging the temperatures of all nodes; instead, a weighted average needs to be applied. For linear tetrahedral elements, the average temperature in each element is the average of the four nodes. The overall average temperature is the weighted average of the temperatures in each element, with the weights being the element volumes. The average temperature can be calculated as follows:

$$T_{avg} = \frac{1}{V} \sum_{e=1}^n V^e T_{avg}^e = \frac{1}{V} \sum_{e=1}^n \left(\frac{V^e}{4} \sum_{i=1}^4 T_i^e \right) \quad (9)$$

where e represents the e -th element and T_i^e represents the temperature of the i -th node in the e -th element.

Maximum temperature gradient: Similarly, for linear tetrahedral elements, the temperature gradient is uniform within each element. The gradient temperature of e -th element can be calculated as:

$$\nabla T^e = \nabla \left(\sum_{i=1}^4 N_i^e(x, y, z) T_i^e \right) = \sum_{i=1}^4 (T_i^e \nabla N_i^e(x, y, z)) = \sum_{i=1}^4 T_i^e [b_i^e \quad c_i^e \quad d_i^e] \quad (10)$$

where $N_i^e(x, y, z) = a_i^e + b_i^e x + c_i^e y + d_i^e z$ represents the i -th basis function of the e -th element.

Since the three objective functions cannot be used directly for optimization, we combine them into a single objective function through weighted summation.

As these three cannot simply be added together, normalization must be performed first: randomly generate a set of different $\mathbf{S}$, and calculate the extremum of the three objective functions for these $\mathbf{S}$. The normalization formula is:

$$x_{norm} = \frac{x_{max} - x}{x_{max} - x_{min}} \quad (11)$$

Additionally, in order to perform optimization, it is necessary to quantify the positions of the heat sources. The position of a heat source is represented by the index of the first super-element it covers. After completing the above preparations, it is necessary to select a discrete multi-variable optimization algorithm. Several algorithms are available, including genetic algorithm (GA), particle swarm optimization (PSO), simulated annealing (SA), and Bayesian optimization (BO), among others. This paper will compare the advantages and disadvantages of these algorithms in Section 4.

4. Experiment

In the experiment, the fundamental parameters of the 3D IC model are shown in Table 1. Five heat sources are set with parameters shown in Table 2. For the convenience of calculation, the heat sink and substrate are set as heat flux boundary conditions with heat transfer coefficients of $35000 \text{ W}/(\text{m}^2 \cdot \text{K})$ and $5 \text{ W}/(\text{m}^2 \cdot \text{K})$, respectively. The surrounding areas are considered as thermal insulation boundary conditions.

Table 1: Parameter of 3D IC Model

Parameter	Value
m, m_x, m_y, m_z	75, 5, 5, 3
Distance between super-elements: d (μm)	40
Height, radius of TSV: h_{TSV}, r_{TSV} (μm)	40, 8
Height, radius of mirco bump: h_{MB}, r_{MB} (μm)	24, 15
h_1, h_2, h_3, h_4 (μm)	5, 3, 1, 3
Thickness of SiO_2 : t_{ox1}, t_{ox2} (μm)	1, 1

Table 2: Parameter of Heat Source

Heat source	S_1	S_2	S_3	S_4	S_5
Size $a_i \times b_i$	1×1	1×2	2×2	2×3	3×3
Power Q_i (mW)	1.6	1.6	3.84	1.92	4.32

Before optimizing the positions of the heat sources, it is necessary to verify the accuracy of the super-element method and estimate its computational time. We use the computational results from COMSOL as a benchmark to validate our algorithm. To ensure the comparability of results, the mesh in COMSOL is set to linear.

After the experiments, the results obtained from the super-element method show a root mean square error (RMSE) of 4.58×10^{-4} compared to COMSOL. Given that the model temperature is around 300 K, this error can be considered negligible. Additionally, the computational time of COMSOL is 125 seconds, while the computational time of the super-element method is 33 seconds. It can be seen that the super-element method significantly reduces the computational cost.

After validating the super-element method, we first use the method mentioned in Section 3.2 to compute the temperature data under the heat source of any single super-element, allowing us to quickly obtain the objective function for arbitrary $\mathbf{S}$. Here, the weights of maximum temperature, average temperature and maximum temperature gradient are set to 0.5, 0.25, and 0.25, respectively. Then, we apply the optimization algorithm mentioned in Section 3.3 to optimize the positions of the heat sources, and the results are shown in Table 3.

To quantify the results after optimization, it is not appropriate to directly compare the maximum and average temperatures before and after optimization; instead, the temperature rise relative to ambient temperature should be considered. According to Table III, the results of the SA algorithm yield the best results, with the maximum temperature rise, average temperature rise, and temperature gradient reduced by 4.58%, 0.64%, and 3.78%, respectively, compared to the average results generated by random positioning of heat sources.

Table 3: Comparison of Optimization Algorithm

Optimization algorithm	GA	PSO	SA	BO
Obtained objective function	0.968	1.024	1.054	0.902
Maximum temperature (K)	360.94	360.76	360.62	361.16
Average temperature (K)	356.83	356.64	356.56	357.04
Maximum gradient (K/mm)	14.31	14.05	13.28	14.96

5. Conclusion

This paper proposes an optimization method for multiple heat source positions in the TSV array scenario of 3D ICs, with the goal of minimizing both the temperature and temperature gradient within the model. To perform thermal simulations at an acceptable computational cost, the super-element

method is employed, leveraging the periodicity of the TSV array to reduce the computational time by a factor of 26.4% compared to COMSOL. Additionally, to quickly obtain the model's objective function for different heat source positions, a multiple heat source simulation algorithm based on the superposition principle is used. Finally, this paper compares the optimization results of various optimization algorithms on the objective function and ultimately selects the SA algorithm. Based on the experiments, the proposed optimization method can effectively reduce the temperature within the TSV array and provide valuable insights for the design of 3D ICs.

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