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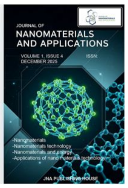

Investigation of Thermal Transport Phenomena in Micro-scale Heat Sinks: Influence of Geometric Architecture and Advanced Material Selection for Nano-electronic Cooling

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Abstract: This study investigates the hydrothermal performance of semiconductor heat sinks through a steady-state Conjugate Heat Transfer (CHT) model utilizing the Finite Volume Method. By examining thermal boundary layer dynamics at the micro-scale interface, the research evaluates the synergistic effects of geometric architecture and material properties. Numerical results demonstrate that copper (Cu) configurations achieve a 2–5 K reduction in base temperature compared to aluminum and Al–Si alloys under equivalent constraints. Circular fin geometries exhibit a 6–10% enhancement in heat dissipation efficiency over square and triangular designs, attributed to optimized effective contact area and streamlined convective flow. Furthermore, increasing fin thickness significantly improves conductive transport, whereas geometric transitions to non-circular profiles exacerbate thermal resistance. These findings provide a robust computational framework for integrating advanced nanomaterials into high-power density cooling systems, establishing a scientific basis for optimizing next-generation nano-electronic thermal management.

Keywords: Heat sink, shape, material, size, heat transfer, COMSOL Multiphysics

1. Introduction

In the context of the rapidly developing microchip and electronics technology, controlling the operating temperature of semiconductor chips has become one of the most important technical challenges [1-3]. The heat generated during chip operation, if not effectively controlled, can lead to overheating, causing performance degradation, shortening device lifespan, and even serious damage. To solve this problem, heat sinks have been researched, developed, and widely applied as a mechanical solution to transfer and dissipate heat into the surrounding environment. A heat sink is a technical component designed to increase the surface area in contact with air, thereby improving the efficiency of heat transfer from the surface of the heat source usually microprocessors or high-power electronic devices to the environment. Common materials used to manufacture heat sinks are aluminum and copper, thanks to their high thermal conductivity and good machinability. According to research by Tuckerman and Pease (1981), the use of micro-grooves in the heat sink structure can increase heat transfer efficiency many times, opening a new direction for micro-heat dissipation [4]. The applications of heat sinks are not limited to the microchip industry but extend to consumer electronics, renewable energy systems, electric vehicles, and data centers [5, 6]. In these systems, optimizing the shape, material, and size of heat sinks plays a crucial role in improving cooling efficiency and equipment durability. However, current studies often overlook the interaction between complex geometry and surface thermal resistance at the nanoscale. This study fills this gap by evaluating fin shape optimization integrated with advanced material properties to meet high-density heat dissipation demands in the nano-electronics era. Besides, the simultaneous influence of these factors under natural convection conditions has not been fully clarified, especially for small and medium power semiconductor chips. In recent years, many studies have focused on analyzing and optimizing heat sinks under natural convection conditions through numerical simulation and experiments. The results show that geometric shape, fin arrangement, and fabrication material have a significant influence on temperature distribution and convective heat transfer coefficient [7-9]. In high-temperature environments, such as data centers, the arrangement and optimization of heat sinks for each device is a decisive factor in sustainable operation and energy saving. According to Lasance (2005), heat dissipation efficiency plays a role of 60–70% in maintaining the operational stability of high-power electronic systems [10]. Regarding manufacturing methods, many technologies are currently used to produce heat sinks, including aluminum extrusion, CNC machining, die casting, and 3D metal printing technology. Each method offers its own advantages, such as aluminum extrusion allowing mass production at low cost, while 3D metal printing allows the creation of complex geometries optimized for heat convection. Garimella et al. (2004) showed that microstructure designs created using 3D printing technology can increase the contact area and heat transfer efficiency by up to 45% compared to traditional designs [11]. Recent research results also show the great potential of optimizing the shape and material of heat sink fins. Bar-Cohen and Kraus (1999) summarized advances in thermal simulation, showing that optimizing the geometry of fins (in terms of height, thickness, and distance between fins) can significantly improve the heat exchange coefficient, while reducing mass and production costs [12]. In addition, Zhang and Peterson (2006) also successfully experimented with micro heat pipes integrated with heat sink fins, improving heat dissipation efficiency in confined spaces [13]. The above results show that heat sink fins are an indispensable technical component in the cooling system of modern semiconductor devices. In-depth research on materials, geometry, and fabrication methods of heat sinks is not only of academic significance but also brings great practical application value, especially in the context of recent research focusing strongly on optimizing shape and natural convection for high-efficiency passive cooling systems [8, 9, 14]. However, previous studies mainly focused on either material selection or geometric optimization separately. A comparative nonlinear numerical investigation considering shape, material type, and thickness simultaneously under natural convection remains limited.

2. Materials and Methods

The numerical investigation in this study is founded on a steady-state Conjugate Heat Transfer (CHT) framework. The implementation of the Finite Volume Method (FVM) allows for a robust discretization of the governing conservation equations, ensuring high accuracy in modeling complex fluid-thermal interactions at the micro-scale [15-17]. This approach has been widely validated in recent literature for predicting temperature distributions and heat flux in advanced electronic cooling architectures.

2.1. Mathematical Modeling and Numerical Method

This study uses COMSOL Multiphysics® 6.1 software to simulate the heat dissipation capability of semiconductor chip heat sinks under natural heat transfer conditions. To do this, we initially built geometric models of the heat sink (circle, square, equilateral triangle) using COMSOL's Geometry tool. In this study, all geometrical models are constructed based on ideal CAD representations. Manufacturing-related imperfections such as surface roughness, dimensional tolerances, and internal defects are not included in the simulations. This assumption allows for a clearer evaluation of the intrinsic effects of geometric shape, material properties, and fin thickness on heat transfer performance. To simulate the heat sink, use the parameters of each metal and alloy listed in Table 1, based on data from Incropera and DeWitt [18].

Table 1. Thermophysical properties of materials at 298 K

Materials	**k (W/m·K)**	**ρ ($\mathrm{kg/m^3}$)**	**c (J/kg·K)**
Copper (Cu)	385	8960	385
Gold (Au)	315	19300	129
Aluminum (Al)	205	2700	897
Al–Si alloy	150	2650	850

Next, we established the air environment surrounding the heat sink. For this problem, we combined the heat transfer and natural convection problem solved using the finite element method [19]. The boundary conditions [20, 21] and grid were set to optimal by fine-tuning the grid at interfaces with large temperature gradients with the fin temperature set at 363 K, ambient air temperature 298 K at atmospheric pressure (1 atm). To ensure numerical accuracy, a mesh refinement strategy was applied with increased mesh density in regions exhibiting high temperature gradients, particularly near the solid–fluid interfaces and fin surfaces. A grid independence study was conducted by comparing simulation results across multiple mesh sizes. The variation in base temperature between successive mesh refinements was found to be less than 1%, indicating that the solution is independent of the mesh size. Therefore, the selected mesh configuration provides a reliable balance between computational cost and accuracy [22]. The heat transfer simulation model is determined by equation (1) in the form:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q \qquad [18] \qquad (1)$$

Q is the heat energy released by the semiconductor chip.

With the heat transfer rate: $q = hA(T_s - T_\infty)$ [18] (2)

and heat dissipation performance is determined by the formula $\eta = Q_0/Q_{max}$ (3)

In this study, the convective heat transfer coefficient (h) is not assumed to be a constant. Instead, it is implicitly determined through the numerical solution of the coupled Navier–Stokes and energy equations under natural convection conditions. This approach allows the local heat transfer coefficient to vary spatially depending on the temperature field and buoyancy-driven airflow. Therefore, the value of h is effectively obtained from the simulation results rather than prescribed a priori, ensuring a more physically realistic representation of natural convection. Where: ρ is the density (kg/m^3), c is the specific heat capacity (J/kg·K), k is the thermal conductivity (W/m·K), h is the convective heat transfer coefficient ($W/m^2 \cdot K$), T_s is the surface temperature, T_∞ is the ambient temperature, A is the heat transfer surface area (m^2), Q_0 is the actual heat dissipation amount, Qmax is the ideal heat amount if the entire fin surface is at the same base temperature. In which, the values of T_s and T_∞ are automatically extracted from the simulation results in COMSOL Multiphysics through the Derived Values tool [19]. With natural convection, at the surface of the simulation model, the Navier–Stokes equations are implemented according to heat transfer (Holman, 2010) [23].

2.2. Governing Equations and Nonlinear Mathematical Model

The heat transfer process in the finned heat sink under natural convection conditions is governed by a coupled nonlinear system consisting of the Navier–Stokes equations and the energy conservation equation. The airflow around the heat sink is assumed to be incompressible, laminar, and driven by buoyancy forces induced by temperature gradients. The governing equations can be written as follows:

$$\nabla \cdot u = 0, \qquad (4)$$

$$\rho(u \cdot \nabla)u = -\nabla p + \mu \nabla^2 u + \rho g \beta (T - T_0), \qquad (5)$$

$$\rho c_p (u \cdot \nabla T) = k \nabla^2 T, \qquad (6)$$

where u is the velocity vector, p is the pressure, T is the temperature, ρ is the fluid density, μ is the dynamic viscosity, c_p is the specific heat capacity, k is the thermal conductivity, β is the thermal expansion coefficient, and T_0 is the ambient temperature. The nonlinearity of the mathematical model arises from the convective terms $(u \cdot \nabla)u$ and $(u \cdot \nabla T)$, as well as from the buoyancy coupling between the momentum and energy equations. Consequently, the thermal performance of the heat sink is strongly dependent on geometric parameters, material properties, and boundary conditions, leading to a nonlinear relationship between the fin configuration and the resulting temperature distribution. In this model, radiant heat transfer is ignored because the operating temperature of the system is not too high. Air convection is assumed to be natural convection in laminar flow mode. These assumptions are consistent with the actual operating conditions of small and medium power semiconductor chips. The results obtained are used to evaluate and compare the influence of shape, size, and material on the heat transfer efficiency of semiconductor chip heat sinks. It should be noted that neglecting manufacturing-induced geometric deviations may lead to slight overestimation of heat transfer performance. In real applications, such imperfections can influence local airflow structures and thermal resistance, particularly under natural convection conditions.

3. Results and Discussion

3.1. Characteristic Quantities of Heat Transfer of Semiconductor Chip Heat Sinks.

To study the characteristics of the heat transfer of semiconductor chip heat sinks, a square heat sink made of copper (Cu) with dimensions of 50 × 50 × 25mm, with longitudinal grooves and a central groove, was selected. The numerical results presented in this section are based on mesh-independent solutions, ensuring that the observed thermal trends are not affected by discretization errors.

The results are shown in Figure 1.

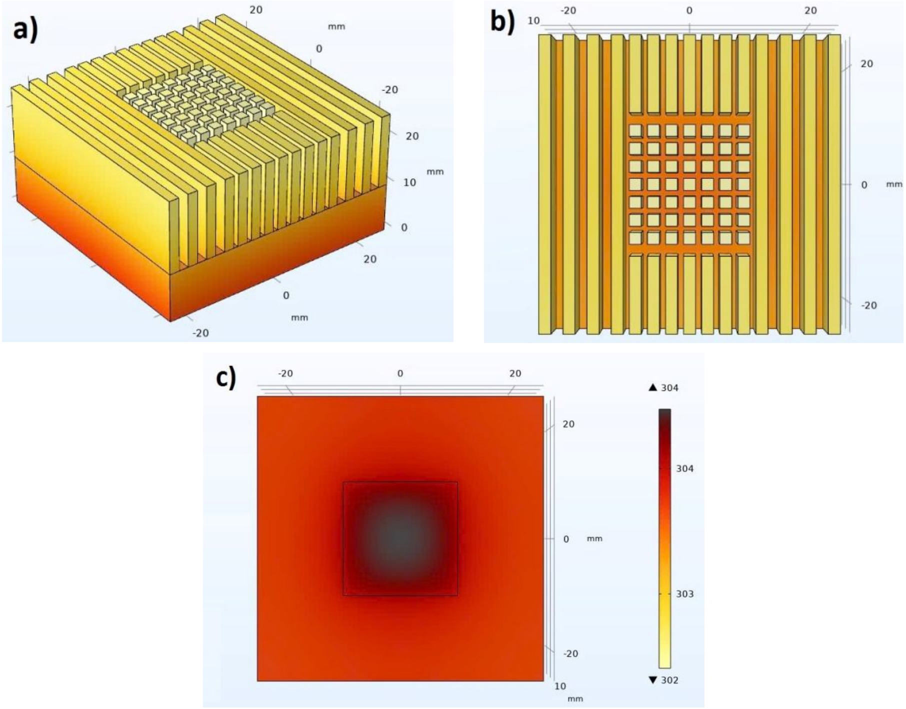


Figure 1 The heat transfer characteristics of a square heat sink with copper material: 3D shape (a), top surface shape of the heat sink (b), bottom surface shape, with temperature column (c) representing the temperature difference of the heat sink at an ambient temperature of 298 K (25°C).

Simulation results show that a square copper (Cu) heat sink with dimensions of 50 × 50 × 25mm and a vertical groove system has the ability to distribute heat relatively evenly. The temperature at the base surface reaches approximately 304 K, while the average temperature on the surface of the fin decreases to approximately 302 K, creating a temperature difference $\Delta T \sim 2\ \mathrm{K}$. This confirms that high thermal conductivity enhances heat transfer efficiency (Figure 1a, 1b). The heat sink structure with vertical fins increases the contact area between the semiconductor chip and the air environment, thereby improving convection and heat transfer efficiency. Increasing the number of fins increases the heat exchange surface area, contributing to improved cooling compared to designs with fewer fins. The material used is copper (Cu), which has a high thermal conductivity of up to 385 W/m·K aligning with recent high-impact studies on graphene-enhanced and high-purity metallic thermal spreaders [24, 25].

The superior heat diffusion rate of copper effectively reduces localized hotspots, which is a critical requirement for maintaining the reliability of nano-electronic devices. Thanks to this property, copper has good heat absorption and conduction capabilities, allowing the material to quickly absorb and transfer heat from the substrate surface to the heat sink fins, thereby reducing the temperature of the semiconductor chip. The substrate surface temperature is the temperature absorbed by the heat sink fins from the semiconductor chip, at 304 K (equivalent to 31 °C), and the heat sink fin temperature is the temperature radiated to the environment, at 302 K (29 °C) (Figure 1c). With a temperature difference between the base, this shows that the heat transfer efficiency of copper is very good. This indicates that this design ensures a balance between heat dissipation and thermal conductivity. Overall, the heat sink design studied shows effective heat distribution and conduction under natural convection conditions. Using copper material will provide high heat dissipation efficiency, but weight and production costs need to be considered. The large number of grooves increases cooling efficiency, but it also needs to be designed appropriately to avoid obstructing the flow of hot air. All these factors need to be carefully considered to achieve an optimal balance between performance, cost, and system durability. This configuration is used as a reference case in subsequent analyses. This square copper heat sink as the basis for studying the factors affecting the heat transfer process.

3.2. Influence of semiconductor chip heat sink factors on heat transfer process

3.2.1. Influence of material.

To study the influence of material by changing from copper (Cu) to gold (Au), aluminum (Al), and Al–Si alloy, the results are shown in Figure 2. Initially, with copper (Cu) material, dimensions: length 50mm, width 50mm, height 25mm, groove thickness 2mm, center cylinder thickness 2mm, outer groove 2mm, inner groove 1mm, number of grooves 15, copper (Cu) thermal conductivity coefficient 385 W/m·K (Figure 2a1, 2b1), base temperature 304 K, heat sink temperature 302 K (Figure 2c1).

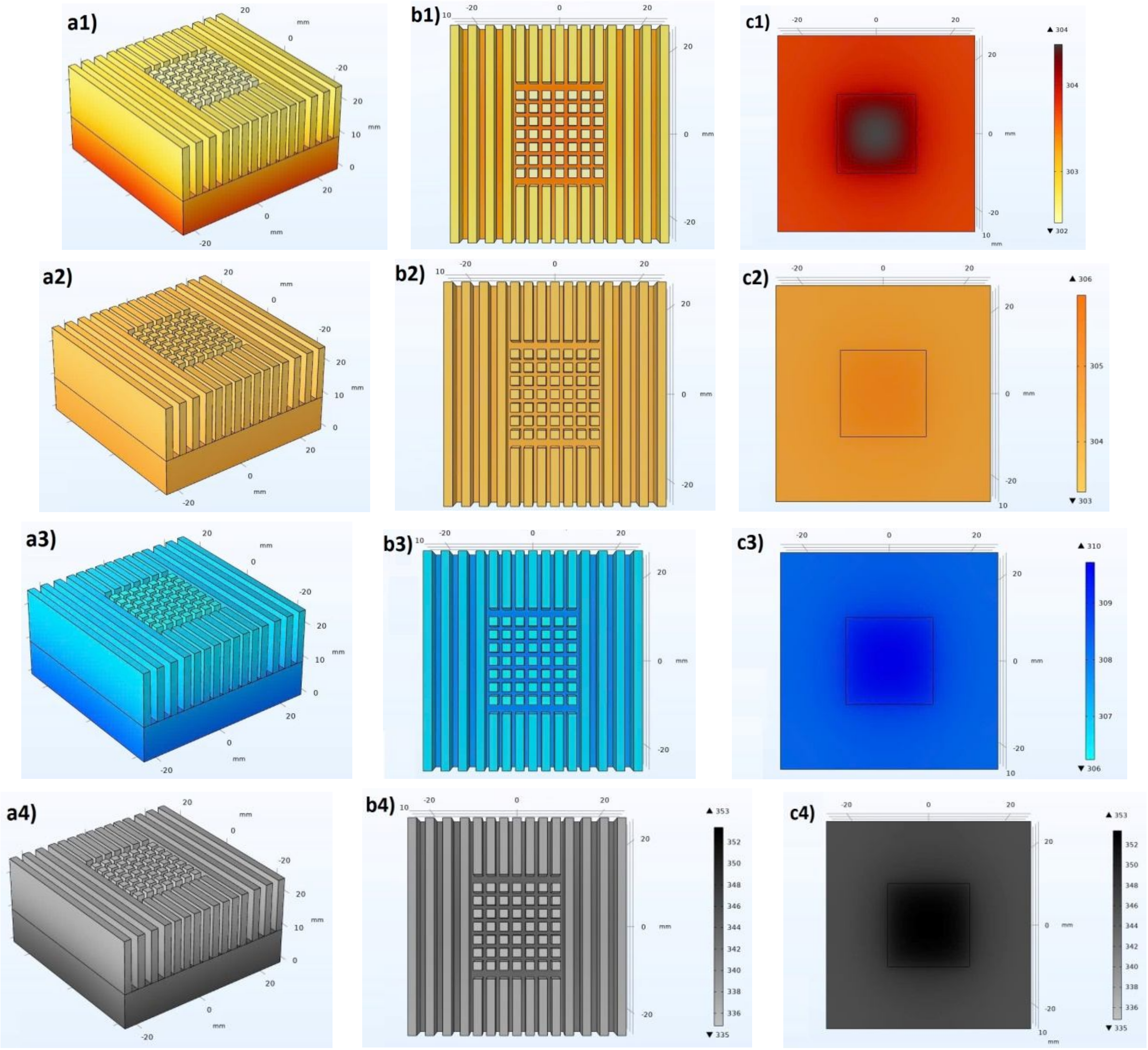


Figure 2 The heat transfer characteristics of copper (a1, b1, c1), gold (a2, b2, c2), aluminum (a3, b3, c3), and Al–Si alloy (a4, b4, c4) at room temperature 298 K.

When replacing copper with other materials such as gold (Figures 2a2, 2b2, 2c2), aluminum (Figures 2a3, 2b3, 2c3), and Al–Si alloy (Figures 2a4, 2b4, 2c4) with the same size and shape, groove thickness, central groove axis and inner and outer groove slots, and number of grooves, the thermal conductivity coefficient of gold is 315 W/m·K, of aluminum is 205 W/m·K, and of Al–Si alloy is 150 W/m·K. The results show that the base temperature increased from 304 K to 306, 310, 353 K and the heat sink temperature increased from 302 K to 303, 306, 335 K (Figures 2c1, 2c2, 2c3, 2c4). The observed increase in temperature reflects the decrease in heat transfer efficiency as the thermal conductivity of the material decreases (Figures 2a1, 2a2, 2a3, 2a4 and Figures 2b1, 2b2, 2b3, 2b4). The observed increase in base temperature with decreasing thermal conductivity can be attributed to the increased thermal resistance within the fin body, which limits axial heat conduction from the base to the fin surfaces. As a result, materials with lower thermal conductivity exhibit localized heat accumulation near the base, reducing overall heat sink effectiveness under natural convection. Given the scope of this research, we decided to choose copper as the basis for studying the influencing factors, as copper meets all the practical requirements [26, 27].

To further clarify the factors directly affecting the heat dissipation process of the heat sink, we continued to study the influence of shape on the heat dissipation process.

3.2.2. Influence of Shape.

To study the influence of shape on heat transfer by changing the shape of the copper material from a circular shape to an equilateral triangle and a square, the results are shown in Figure 3.

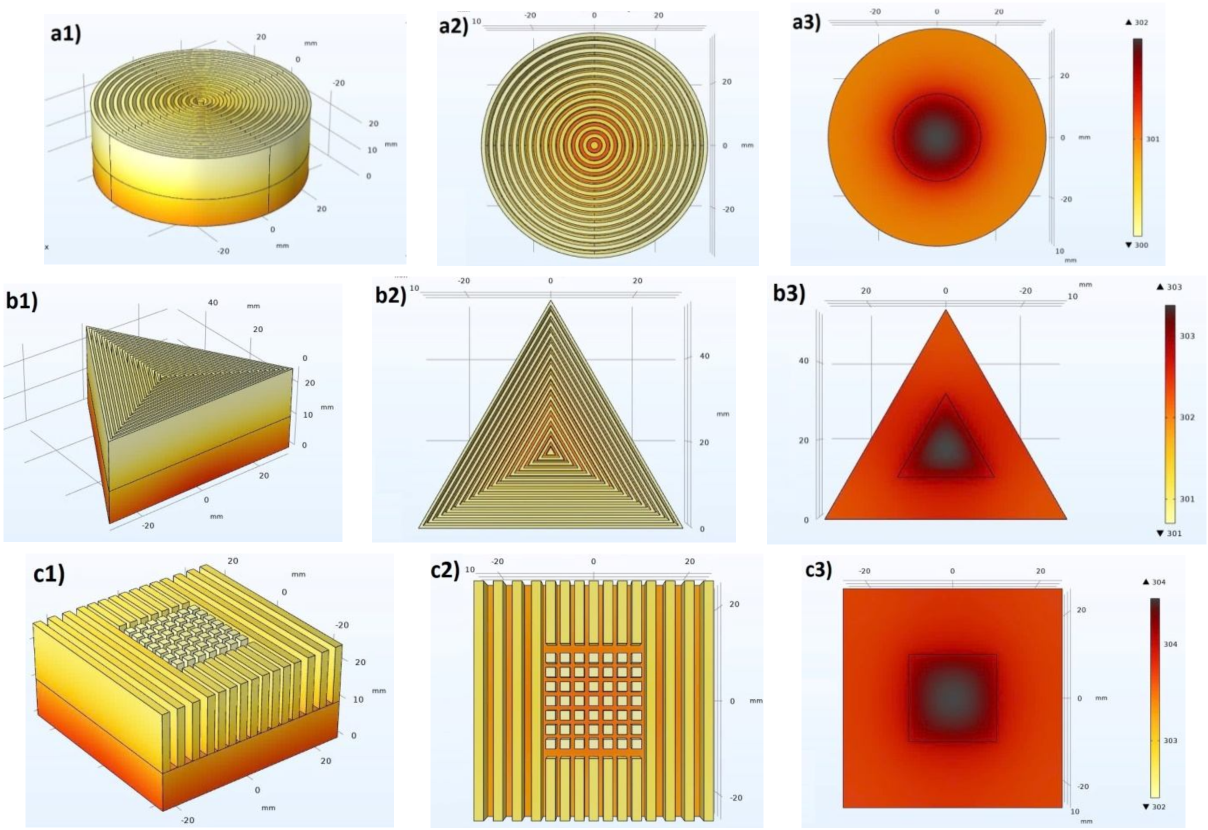


Figure 3 The heat dissipation characteristics of Cu with different shapes: circular (a1, a2, a3), equilateral triangle (b1, b2, b3), square (c1, c2, c3) at 301 K.

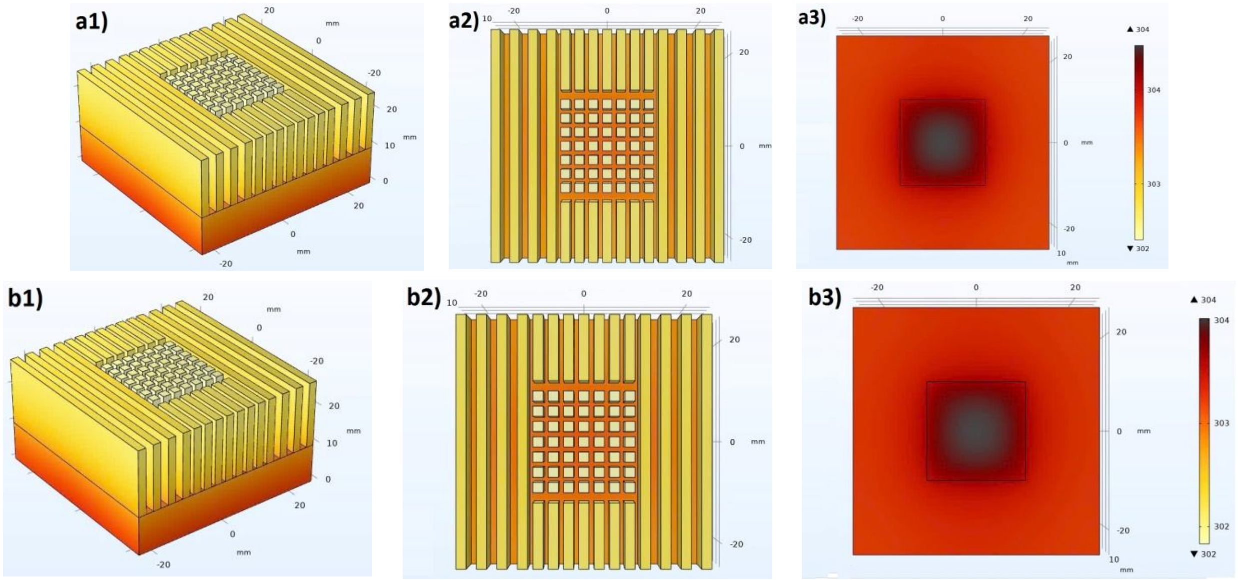
The results show that, with Cu heat sink material having a thermal conductivity of 385 W/m·K, changing the shape from circular to equilateral triangle and square leads to a decrease in the surface area of the heat sink base in contact with the semiconductor chip. Within the same outer dimensions, the circular shape provides more uniform heat distribution and symmetric airflow patterns compared to square and triangular shapes. In this case, the heat sink has a temperature range that transfers heat from the base to the fins and to the outside air with a temperature range varying from 302 K to $300\ \mathrm{K}$ ($\Delta\mathrm{T}\ \sim 2\ \mathrm{K}$) in a circular shape (Figures 3a1, 3a2, 3a3), a square shape from 304 K to 302 K (Figures 3b1, 3b2, 3b3) and an equilateral triangle shape from 303 K to 301 K (Figures 3c1, 3c2, 3c3). In addition to the effective contact area, the circular geometry promotes a more symmetric airflow pattern around the heat sink, reducing stagnant zones and enhancing buoyancy-driven convection. In contrast, sharp corners in square and triangular fins tend to induce localized flow separation, which slightly deteriorates convective heat transfer efficiency. This shows that the heat dissipation capacity of the heat sink is always directly proportional to the surface area in contact with the environment. Circular shapes have the largest surface area, square shapes have a larger surface area than equilateral triangles but a smaller surface area than circular shapes. The results show that circular heat sinks have the lowest base temperature, followed by square and equilateral triangle shapes, reflecting the role of effective contact area in improving heat transfer efficiency as circular geometries facilitate a more streamlined flow and minimize the formation of large wake regions behind the fins [28, 29].

This structural advantage results in a higher Nusselt number and enhanced convective heat transfer coefficients compared to traditional square or rectangular designs. This trend is also consistent with recent studies on natural convection heat sinks, where configurations with large effective contact areas and symmetrical airflow distribution show superior heat dissipation performance compared to shapes with many angles. CFD simulation and experimental studies have shown that optimizing the shape of the heat sink can reduce the base temperature by 5–15% compared to traditional designs [9, 30].

The above results show that to achieve faster heat transfer, the surface area in contact with the semiconductor chip and the environment needs to be increased. This result indicates that in the design of heat sinks for semiconductor chips operating under natural convection conditions, shapes with a large effective contact area, such as circles, are the preferred choice when high heat dissipation efficiency is required. For cases with limited installation space, a square shape can be considered a balance between heat transfer efficiency and manufacturing feasibility.

3.2.3. Influence of Size.

To study the influence of size on heat transfer by changing the thickness of the heat sink fins by increasing and decreasing the thickness of the semiconductor chip by 2mm, the results are shown in Figure 4.



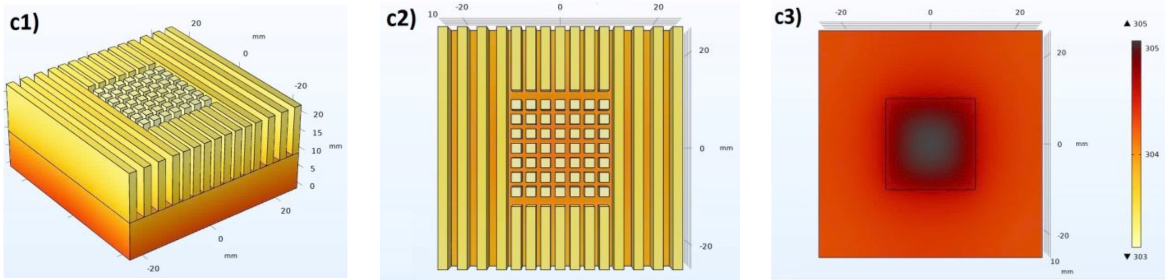


Figure 4 The heat transfer characteristics of Cu heat sinks with different thicknesses: Initial heat sink (a1, a2, a3), heat sink increased by 2mm (b1, b2, b3), heat sink decreased by 2mm (c1, c2, c3) at 301 K.

The results show that, with square Cu material used as a heat sink with a thermal conductivity of 385 W/m·K, the temperature range is from 304 K to 302 K (Figure 4a1, 4a2, 4a3). When the thickness is increased by 2mm, this temperature range does not change (Figure 4b1, 4b2, 4b3). When the thickness is decreased by 2mm, the temperature range is from 305K to 303K (Figure 4c1, 4c2, 4c3). In this study, the temperature difference between the base surface and the heat sink is equal to $\Delta \mathrm{T} \sim 2\ \mathrm{K}$. However, the temperature at the base surface increases with decreasing thickness, indicating that reducing the thickness of the heat sink actually increases the base temperature. This is because it depends on the heat absorption capacity of the base. If the base has good heat absorption, the base temperature will be lower, and vice versa. Increasing the thickness of the heat sink tends to improve heat transfer under the studied conditions. This shows that the thickness of the heat sink directly affects the absorption and distribution of heat from the base, especially under natural convection conditions.

3.3. Nonlinear Effects of Geometric Parameters

From a mathematical perspective, the obtained results indicate a nonlinear dependence between the geometric parameters of the heat sink fins and the maximum base temperature. Small variations in fin shape and thickness lead to disproportionate changes in the thermal response, confirming the strongly nonlinear nature of the coupled flow and heat transfer problem. This behavior is consistent with nonlinear convection–diffusion systems reported in recent studies on natural convection heat sinks [7, 9, 14]. This nonlinear behavior highlights that fin optimization cannot be achieved through linear scaling of geometric parameters, emphasizing the necessity of numerical optimization in practical heat sink design. Furthermore, the present analysis is based on idealized geometries. In practical manufacturing processes such as extrusion, machining, or additive manufacturing, surface irregularities and geometric deviations may arise. These factors can alter local heat transfer behavior and should be considered in future studies through experimental validation or reconstructed geometries from techniques such as 3D scanning or computed tomography. Although the temperature differences observed in this study are relatively small (on the order of ~2 K), such variations can still be practically significant in semiconductor applications. Even slight reductions in operating temperature can enhance device reliability, reduce thermal stress, and extend service life, particularly under continuous operating conditions. The numerical dataset generated in this study also has potential applications beyond conventional analysis. Specifically, it can be used as training data for surrogate models, such as artificial neural networks, to predict thermal performance as a function of geometric and material parameters. Such data-driven approaches can significantly reduce computational cost by replacing repeated finite element simulations with fast predictive models. This is particularly relevant for optimizing nonlinear design parameters of heat sinks under natural convection conditions and aligns with recent trends in computational engineering.

4. Conclusion

This study systematically evaluated the thermal performance of heat sinks as a function of geometric architecture, material properties, and fin thickness. Numerical results demonstrate that copper (Cu) exhibits superior heat dissipation efficiency, followed by gold, aluminum, and Al–Si alloys, due to its enhanced thermal conductivity. Circular configurations outperformed square and equilateral triangular designs by optimizing the effective contact area and streamlining natural convection flow. Furthermore, increased fin thickness significantly improved conductive transport, whereas thickness reduction exacerbated substrate thermal resistance. The findings indicate that integrating nano-carbon coatings or graphene-based composites could further mitigate thermal bottlenecks in Cu-based circular models, representing a promising frontier for next-generation, high-power density semiconductor thermal management. While these results, supported by grid independence verification, provide robust design guidelines for passive cooling in electronic packaging and renewable energy systems, they are derived from idealized geometries. Future research should prioritize experimental validation using advanced thermography and investigate the influence of manufacturing-induced imperfections on micro-scale thermal transport. These conclusions align with contemporary trends in passive cooling optimization, emphasizing the synergistic role of material selection and geometric design in enhancing efficiency.

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