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# Simulation of matrix conductivity in copper–diamond composites sintered by field assisted sintering technology

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ABSTRACT

This research investigates thermal conductivity properties of Cu/Zr alloys combined with diamond particles to form a composite that possess superior thermal conductivity. This article describes the use of a theoretical calculation and finite element analysis to compare to previously published experimental observations. Both theoretical calculations and finite element analysis indicate that experimental results cannot be explained solely by an improved interface between the matrix and diamond particles, as originally suggested. This study shows that the experimental results, theoretical calculations, and finite element analysis are in agreement when the thermal conductivity of the matrix is adjusted to compensate for the amount of zirconium lost to the interface. This finding can be used to predict the thermal conductivity of a composite material composed of a Cu/Zr matrix with diamond particles.



## 1. Introduction

Thermal management is a critical issue in the development of high performance semiconductor devices that are used in radar, satellites, and other power intensive electronics. Heat sink plates are attached to semiconductor chips to dissipate the heat that they generate. The major issues that face the development and inclusion of heat sink plates into electronic packages are heat dissipation and thermal stress. Poor heat sink performance can limit the performance and lifetime of the device.

The trend in power electronics is to decrease the geometric size of the chip and simultaneously increase the power. The combination of these factors leads to a significantly increased current density and higher heat generation. If the extra heat is not dissipated, it will limit the performance and/or lifetime of the die. Heat sink performance must be improved to accomplish the goal.

One common approach to solving this problem is to tailor the material composition of the heat sink to have more desirable properties by blending two or more different materials that have desirable properties. Copper–diamond is an attractive combination due to the high thermal conductivity and the low coefficient of thermal expansion (CTE) of diamond. However, the large CTE difference and lack of chemical reactivity between copper and diamond both contribute to a poor interface between the copper matrix and diamond particles. The poor interface gives rise to inefficient thermal transport and an ultimate reduction in thermal conductivity observed in the composite material.

Numerous studies have been done on copper–diamond composite materials to improve the copper–diamond interface, which has been shown to be critical in the thermal performance of the composite. These approaches involve using an additional element to act as a coupler between diamond and matrix. The coupler material is either added as coating on the diamond particles or as an alloying element in the matrix. Several studies use diamond particles coated with a carbide forming element as the starting point to create a strong interface. Another approach is to use an alloy containing the carbide forming element. In both cases, the carbide forming element can react with the diamond to create a better interface for more efficient heat transfer [1–7].

Limited research has been completed on thermal simulations of these composite materials. One of these studies uses a Diffuse Mismatch Model (DMM) as a theoretical model for the thermal conductivity of the composite material. The authors assume that the thermal conductivity of the matrix is 330 W/m K [7]. This value is significantly higher than the values that were experimentally determined in previous research [8].

Another work applies a simplified acoustic mismatch model (AMM) to calculate the theoretical thermal conductivity of Cu–Ti and Cu–Cr matrix alloys. The results suggest that the interfacial thermal resistance between the matrix and diamond relies heavily

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on material selection and preparation methods. The optimal carbide layer thickness was found to be 0.6–0.9 μm [9].

The other relevant work used Finite Element Analysis (FEA) to simulate aluminum–diamond composites. The authors model the diamond particles as tetrakaidecahedrons. The authors determined that the quality of the interface between the aluminum matrix and the diamond particle is the most important factor in the thermal conductivity of the composite [10].

The objective of this work is to develop a model that accurately describes the nature of the interface of copper–diamond composites created by Field Assisted Sintering Technology (FAST). Additionally, the successful model will allow prediction of composite thermal properties based upon diamond content, interfacial layer thickness, and base alloy composition. The models are designed to describe the experimental results given in previous work [8,11].. The models were built to describe the (near) fully dense systems in the referenced works.

## 2. Experimental details

This research seeks to describe the copper–diamond composite using two methodologies: a Finite Element Analysis (FEA) of a standardized unit of composite material and a thermal circuit analysis using the Diffuse Mismatch Model (DMM) to describe the interfacial losses.

The FEA determines the thermal conductivity by applying a heat source to a unit element of composite material and analyzing the resulting temperature field. Thermal conductivity can be calculated from the thermal resistance, which is defined by Eqs. (1) and (2). The latter equation applies only to one dimensional Cartesian cases.

$$R = \frac{\Delta T}{Q} \tag{1}$$

$$R = \frac{x}{Ak} \tag{2}$$

where $R$ is the thermal resistance, $x$ is the distance between measurement points, $A$ is the cross sectional area, $Q$ is the heat flow rate across the material, and $k$ is the material thermal conductivity. These equations can be combined to solve for thermal conductivity as given in Eq. (3).

$$k = \frac{Qx}{A\Delta T} \tag{3}$$

Eq. (3) shows that the thermal conductivity can determined for any material undergoing a 1D heat transfer if the heat flow rate and temperature difference across the distance $x$ is known. Therefore, the FEA model was designed with a fixed inlet heat rate on one surface and a fixed temperature on the opposing surface. The resulting maximum temperature on the heating surface is then used to calculate the composite thermal conductivity using Eq. (3).

A geometric mode was imported into Ansys Mechanical Heat Transfer Module for thermal simulation, which solves Fourier's 3-dimensional heat equation. The fixed static boundary conditions were chosen and applied to each model so that the thermal conductivity of each assembly could be calculated. A 1 W heat load was applied to one face of the cube. The opposite face of the cube was set to a fixed temperature of 22 °C. The other four surfaces of the cube were set to represent perfect insulation. This creates a one dimensional heat transfer condition to which Eq. (3) can be applied. Fig. 1 shows a schematic diagram of the block and the boundary conditions that were used in the experiment. Material constants were determined from experimental data, where applicable, and are listed in Table 1.

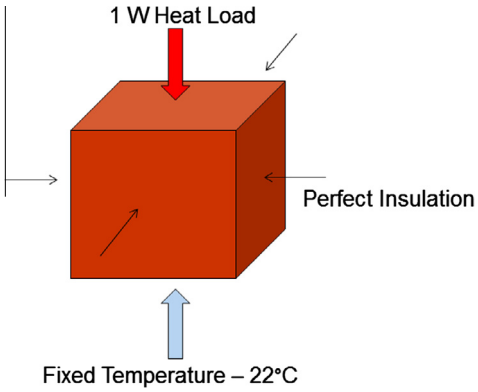


**Fig. 1.** Schematic diagram showing boundary conditions that were used in the simulation.

**Table 1**
Material properties used as input parameters in the thermal models.

| Material | Thermal conductivity (W/mK) |
|---|---|
| Cu (sintered) | 360 ± 36 |
| Diamond | 1200* |
| CuCrZr | 245 ± 25 |
| CuAgZr | 315 ± 31 |
| ZrC | 20* |

* Theoretical value was used.

The solid models for the copper and copper alloy–diamond composite systems were built in Solidworks CAD software package. The diamond particles were assumed to take the shape of a tetrakaidecahedron (14-sides polygon). The diamond particle was created to be 50 μm (17 μm sides) to closely match with the experimental particle size that ranged from 40 to 60 μm. The carbide interface layer was created by adding a 100 nm thick layer directly surrounding and in contact with the diamond surface. Finally, the diamond/interface assembly was centered inside a cube that represents the copper alloy matrix. The size of the cube was chosen so that the diamond particle would occupy the desired volume percentage of the domain. The volume of such a diamond particle was determined to be $5.8 \times 10^{-14}$ m. The cubes were chosen to have volumes of $6.25 \times 10^{-13}$ (side length = 85.5 μm), $3.12 \times 10^{-13}$ (side length = 67.8 μm), and $1.57 \times 10^{-13}$ (side length = 54 μm for 10, 20, and 40 vol.% diamond particles, respec-

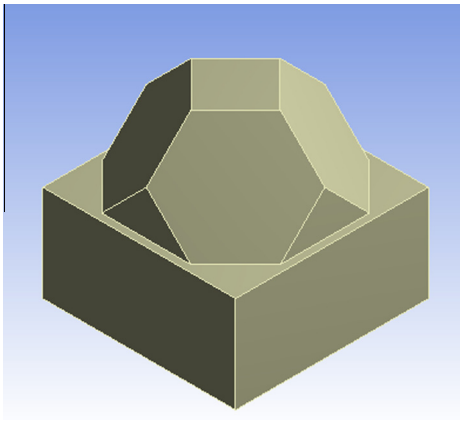

**Fig. 2.** Figure of the diamond-void–matrix model. The figure shows a cross section of the block to expose the diamond model. In this example, the diamond particle occupies 40 vol.% of the total volume of the computational domain.