Journal of Xi'an Shiyou University, Natural Science Edition **ISSN: 1673-064X**

Mathematical investigation of heat transfer model in the solid-carbon/liquid-copper system

Attra Ali[1], Sumaira Yousuf Khan[2]* Fatima Riaz[1]

[1] Institute of Business Management, Karachi, Pakistan
[2] Dawood University of Engineering and Technology, Karachi, Pakistan

*Corresponding Author: Sumaira Yousuf Khan

Abstract: *Through the application of Fourier's law, it is conceivable to examine the thermal conductivity of both carbon and copper fluid with copper-chromium, bringing potentially a promising perspective for the fabrication of materials possessing enhanced thermal transfer properties. In this Research, the estimated thermal conductivity values of a composite established with the Fourier Law will be compared. The research carried out illustrates how the migration of Copper-Chromium (Cu-Cr) from the matrix to the interface modifies the thermal conductivity of carbon/copper (C/Cu) composites. For estimating heat flow values across various Cu-Cr material thicknesses, C/Cu composites were adopted. Heat transfer coefficients have recently been the object of several studies in literature, however, the vast majority of these are based on experimentation with little basic theoretical work available. The challenges encountered in understanding high-temperature and vacuum configurations may be partially responsible for this research gap. A numerical simulation methodology for analyzing heat was introduced in the study. An analytical-numerical simulation framework for the solid carbon/liquid copper-chromium system has been provided in the article.*

Keywords: *Mathematical modeling. Thermal conductivity, Heat flux, Carbon-copper composite, Copper-base alloy*

Introduction

When developing high-performance microelectronic electrical circuits that power many kinds of devices, including radar systems, satellites, batteries, and many other kinds of electronics, efficient control of temperatures is a crucial and fundamental consideration. Recent advancements in technology have enabled the development of tightly packed high-power devices. Additionally, numerous pieces of electrically powered devices generate a lot more heat when they are running than when they are in standby mode [1-5]. As a result of the conventional positive air-cooling approaches are no longer as effective, which has increased the need for cutting-edge thermal management strategies for improving the life expectancy and efficiency of these technological devices. Conduction comprises the fundamental mechanism of passing along heat in technological devices [8-11]. Therefore, it becomes essential to take consideration of essential considerations while constructing an efficient heat sink, such as high thermal conductivity, low coefficient of thermal expansion (CTE), and acceptable machinability [12].

precisely a consequence, materials possessing such characteristics are of the utmost importance for the creation of sustainable temperature control solutions for an assortment of applications. Copper (Cu), which has become renowned for its extraordinary conductivity, stands out as a material that possesses outstanding machinability and financial sustainability. As a result of this, it is a potential decision-making for implementation in thermal management device design [13-15]. It's somewhat reduced mechanical strength, however, precludes this material from possessing a broader spectrum of applications. For developing high-strength and highly efficient temperature control devices, researchers have been investigating the development of composite materials, typically composed of numerous components restricted together through physical or chemical methodologies. For the manufacture of various composite materials with improved heat management capabilities, for illustration, various thermally conductive additives including aluminum (Al), silver (Ag), and others have been implemented as fillers throughout polymer matrices [16-19].

Additionally, copper (Cu)-containing composite materials have been investigated and demonstrated to perform somewhat more effectively when it comes to heat management. Due to the unique combination of high strength as well as suitable conductivity, researchers have demonstrated a particular interest in copper-chromium (C-Cr) and copper/diamond composites. However, their widespread application in large-scale thermal management applications has been restricted by the challenging machinability of Cu/diamond composites and the substantially more impoverished thermal insulation of Cu-Cr [20-22]. The requirement for creative thinking and the creation of novel materials that offer an appropriate combination of high conductivity, improved machinability, superior physical characteristics, and greater endurance is putting put pressure on materials scientists. Due to their enormous surface area, powerful mechanical strength, excellent electrical conductivity, thermal stability, and lightweight, carbonaceous materials are currently gaining an enormous amount of attention.

Carbonaceous materials, that possess the desired dimensional stability along with excellent thermal features, ranging have an extensive variety of makes use of composite materials. Consequently, the creation of composite materials incorporating the characteristics of copper and carbon provides the potential to supply an ideal material that possesses greater conductivity and machinability. We offer a numerical examination that concentrates on a heat transfer model that applies to the solid-carbon/liquid-copper system in this context.

Liquid melt infiltration (LMI) is a popular technique for manufacturing these composite materials. Mathematical modeling has been employed to examine the parameters determining the thermal management performance of these manufactured composite materials. Fourier's law is used to analyze how heat conducts within the composite materials that were previously manufactured [23-24]. It was investigated how the concentration of carbon affected thermal conductivity. Although fullerene soot has a much lower thermal conductivity than carbon nanotube-containing composites, a comparison of the thermal conductivity of Cu-fullerene soot composites and Cu-based composites reported in the literature revealed that the prepared materials are not less thermally conductive than carbon nanotube-containing composites.

Pure copper is regarded as a low strength material although being a common, reasonably priced, and highly conductive substance. Copper compounds with excellent mechanical properties can be produced through alloying, however the conductivity of copper is much decreased. A material with great strength and negligible loss of conductivity can be produced by dispersion hardening. A material's mechanical characteristics can be considerably improved by the incorporation of fullerenes and carbon nanotubes [25].

The ability to characterize heterogeneous materials through brute force analysis is growing more and more prevalent as modern computers' processing capability increases. What was only possible a few decades ago with basic or extremely symmetrical models, especially in 2D, is now possible even with household computers. The representative volume element (RVE) [26], which specifies the minimum size of a representative cell needed to provide attributes of composite material under a specific inaccuracy, is the foundational concept of this accomplishment.

It is now conceivable to simulate sufficiently large RVEs to investigate the characteristics of novel metal matrix composites reinforced with carbon nanofibers (CNF) using computer power, which is already readily available. These are a novel class of engineering materials that provide the opportunity to customize characteristics and satisfy needs, as in heat sinks. For example, because of their low cost, good machinability, small coefficient of thermal expansion, and potential for high electrical and thermal conductivity, CNF-reinforced copper composites are a great choice for use as an electrical contact material and/or substrate for semiconductor devices.

In the context of production and consumption, copper and copper alloys remained one of the most common types of commercial metals, standing in third only to aluminum and iron/steel. Their superior electrical and thermal conductivities, exceptional resistance to corrosion, ease of manufacturing, and durability and fatigue resistance make them frequently utilized. Electrical contacts, cables, wires, and many other components that need to carry electrical current are made mostly of pure copper [27-28].

Nevertheless, because of its substandard mechanical attributes, its use at high temperatures has limitations. Copper's application scope has been broadened by adding hard particles to the matrix, which not only improves mechanical performance and wear resistance but also maintains copper's favorable electrical and thermal conductivity [29]. Compared to pure copper and copper alloys, copper-based composites' high strength, high conductivity, resistance to high temperatures, and wear characteristics are essential and required characteristics for resistant electrodes, electric contact materials, and many other industrial applications [30].

Mathematical Modeling

When favorable conditions have been created, the rate of thermal motion can be monitored for quantifying heat transfer. The rate of thermal transfer through an environment is directly proportional to the negative temperature gradient and the area through which heat moves around, according to Fourier's law. According to the way electrical resistance along electrical conduction has a relationship, heat resistance is precisely inversely proportional to heat conductance. Fundamental concepts in physics and engineering, among them heat conduction describe how heat advances through an environment over time. The concepts are frequently used in various fields of solid-state physics, fluid dynamics, and thermodynamics. Let's examine them more thoroughly in detail:

Just as electrical resistance is related to power conduction, heat resistance is directly proportional to heat conductivity. Thus, heat transmission and thermal resistance are comparable.

[24, 25]. A particular method to characterize heat conduction is Equation A.

Heat Flow = $\frac{\boldsymbol{Difference\ in\ Thermal\ Potential}}{\boldsymbol{Resistance\ to\ high\ Temprature}}$ **(A)**

The thermal potential difference, or temperature change (ΔT) that denotes the difference between the system's internal and external temperatures, can be applied to determine the amount of heat conduction in this context. The system's heating properties are evaluated using thermal resistance. It can be accomplished to calculate this thermal resistance using Equation B.

Resistance to high Temperature = $\frac{\boldsymbol{L}}{\boldsymbol{KA}}$ **(B)**

where L, k, and A are the values for the plate thicknesses, thermal conductivities, and area, correspondingly, in the above formula. Following Fourier's Law, "The rate of heat propagation through a material over a certain period is directly proportional to the negative variation in temperature and to the surface area."

Equation C presents a mathematical representation of the Fourier law.

$$\boldsymbol{q = -k\Delta T} \qquad \textbf{(C)}$$

Here, the terms k, q, and ΔT stand for the material conductivity, temperature difference, and heat flow density, respectively.

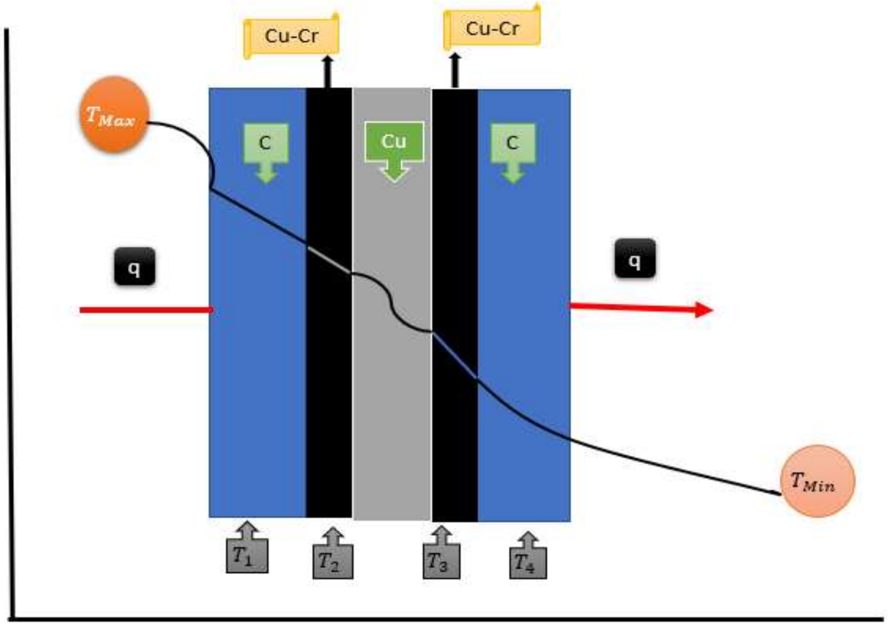

Figure 1: Heat transportation from one material to another material at different temperatures.

We focused on using Fourier's law to determine the transportation of heat in a system consisting of liquid copper and solid carbon. Assume a particular scenario: three plates made of liquid copper and solid carbon are put through to heat. A tiny quantity of Cu-Cr (copper-chromium alloy) is used to join the copper and carbon components.

To attain this goal, we first divided Fourier's rule into three basic parts, which are represented by Equations D through F.

$$\boldsymbol{q_C = -K_A A \frac{T_2 - T_1}{\Delta X_\alpha}} \qquad \textbf{(D)}$$

$$\boldsymbol{q_{Cu} = -K_B A \frac{T_3 - T_2}{\Delta X_\beta}} \qquad \textbf{(E)}$$

$$\boldsymbol{q_{cu-Cr} = -K_c A \frac{T_4 - T_3}{\Delta X_\gamma}} \qquad \textbf{(F)}$$

Equation D shows the heat flux through the carbon fiber, the thickness is expressed by ΔX_α, and the temperature difference indicates the material's thermal potential. The heat flux through the copper material is shown in Equation E, where the thickness is indicated by $\Delta X_\beta$and the temperature change represents the carbon fiber's thermal potential. The heat flux quantities for Copper-Chromium (Cu-Cr) with thickness represented by ΔX_γ are expressed in Equation F. As a result, Equations D through F can be added together to create Equation G, which is the result of adding up all three equations. In the meantime, Equation H is the last formula used to determine the system-wide heat flow, or in other words, Equation H illustrates the simplified form of the Fourier law.

$$\boldsymbol{q = \frac{T_2 - T_1 + T_3 - T_2 + T_4 - T_3}{-\frac{\Delta X_\alpha}{K_\alpha A} - \frac{\Delta X_\beta}{K_\beta A} - \frac{\Delta X_\gamma}{K_\gamma A}}} \qquad \textbf{(G)}$$

$$\boldsymbol{q = \frac{T_4 - T_1}{\frac{\Delta X_\alpha}{K_\alpha A} + \frac{\Delta X_\beta}{K_\beta A} + \frac{\Delta X_\gamma}{K_\gamma A}}} \qquad \textbf{(H)}$$

The process that occurs when thermal energy (heat) passes from some parts of a material that is warmer to a region the fact that is cooler is commonly referred to as heat conduction. It develops because of interactions between atoms in proximity, molecules, or electrons in the material in question. The temperature gradient (difference in temperature between two places) and the material's thermal conductivity are the two parameters that affect the pace of heat conduction.

Result and Discussion

In the present investigation, we implemented Fourier's law within the numerical analysis of heat passing on Copper, which used to be considered as durable, has begun to deteriorate mechanical strength and is no longer a viable option because of this. Our first plan was to find a material that satisfies our requirements for high mechanical strength as well as favorable thermal conductivity. A table featuring individual heat flux values corresponding to different thicknesses of the copper and copper-chromium composite has been generated using the heat flux values from equation H, which characterizes the material's heat flux. Establishing the most appropriate heat flow parameters along with figuring out the importance of thickness in the present scenario are our primary objectives.

A one-meter square area of solid carbon, liquid copper, and Copper-Chromium was fixed in Table 1.

Table 1 demonstrates variations in heat flux based on various Copper-Chromium thicknesses Δx_c, with fixed solid carbon (Δx_α = 10 μm) and liquid copper (Δx_β = 6μm) thicknesses and thermal conductivities of the three materials of solid carbon, liquid copper and Copper-chromium is 1000 W/m-K, 401 W/m-K, and 323.4 W/m-K respectively.

		$\Delta T(K)$			
		10	20	30	40
Δx_γ	0.25	388.566	777.132	1165.679	1554.265
	0.5	377.246	754.570	1131.715	1508.940
	0.75	366.546	733.192	1099.648	1466.184
	1	356.456	712.992	1069.348	1425.784

In this situation, however, Copper Chromium thickness has the reverse consequences, causing an overall decrease in heat flux as it thickens. By observing Table 1, the temperature increment causes an increment in heat conductivity with a corresponding thickness of the copper-chromium alloy, this can be noticed that the thickness of solid carbon, and liquid copper was fixed but the thickness of copper-chromium changes from 0.25 μm to 1 μmat thickness of 0.25 μm the heat conductivity increased from 388.56$6\ w/m^2$ to 1554.265 w/m^2, which is the highest increment of heat flux at temperature difference 40K.

Table 2 depicts variations in heat flux based on various Copper-Chromium thicknesses Δx_c, with fixed solid carbon ($\Delta x_{\alpha} = 10\mu m$) and liquid copper ($\Delta x_{\beta} = 5\mu m$) thicknesses.

		$\Delta T(K)$			
		10	20	30	40
Δx_{γ}	0.25	430.258	860.516	1290.774	1721.032
	0.5	416.408	832.816	1249.224	1665.632
	0.75	403.422	806.844	1210.266	1613.688
	1	391.221	782.442	1173.664	1564.885

In above Table 2, the thickness of liquid copper is reduced by one unit from $6\mu m$ to $5\mu m$, and the result can be analyzed as per the change in heat flux increased with an increment of temperature difference from 10K to 40K, the maximum value of heat flux observed was at $0.25\mu m\ the$ thickness of copper-chromium and at a temperature difference of 40K which is 1721.032.

Table 3 exhibits variations in heat flux based on various copper-chromium thicknesses Δx_{γ}, with fixed solid carbon ($\Delta x_{\alpha} = 10\mu m$)and liquid copper ($\Delta x_{\beta} = 4\mu m$)thicknesses.

		$\Delta T(K)$			
		10	20	30	40
Δx_{γ}	0.25	481.971	963.943	1445.915	1927.887
	0.5	464.659	929.319	1393.978	1858.638
	0.75	448.547	897.095	1345.643	1794.190
	1	433.515	867.031	1300.547	1734.063

The heat flux values displayed in Tables 1, 2, and 3 have been employed to optimize the thickness of the copper composite concerning deviations in copper-chromium thickness by using a simplified form of the Fourier law equation H.

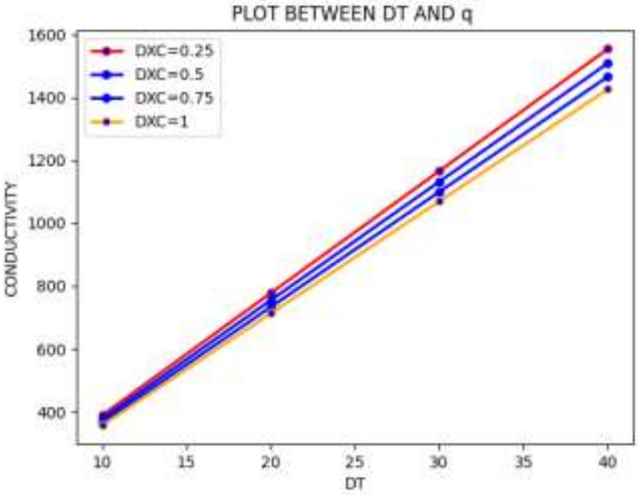

Figure 2: Graphical representation of heat flux when the thickness of liquid copper is Δx_{β} = 6μm

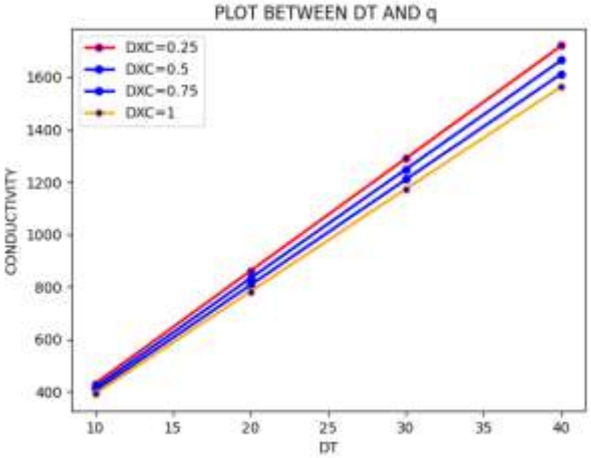

Figure 3: Graphical representation of heat flux when thickness of liquid copper is Δx_{β} = 5μm

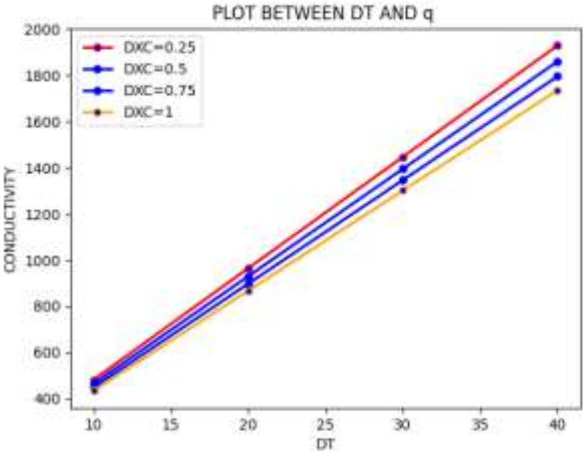

Figure 4: Graphical representation of heat flux when the thickness of liquid copper is Δx_{β} = 4μm.

Figures from 2- 4 represent the graphical increment of the heat flux, as it can be seen through all three graphs that the slope is positive and conductivity is continuously increasing with increment in temperature. The above graphs showed that as the thickness of liquid copper decreased from 6-micron meters to 4-micron meters the conductivity increased from 1600 w/m-k to 2000 w/m-k. The results indicate the change in thickness is caused by to change in heat transformation or heat conductivity, as it can be seen through the observation that the thickness directly affects the thermal change in material, this cause may represent the relationship between the material and the epoxy which make the material to be bonded strongly with each other. Another important observation that can be analyzed here is that each table has a different thickness of material, and each thickness also affects the heat conductivity, and on the other hand temperature fluctuation has a big impact on conductivity.

Conclusion:

The thermal conductivity of a composite constructed from solid carbon and liquid copper was extensively investigated computationally in this research undertaking, with copper-chromium functioning as the thermal interface interconnecting these two materials. To put together a composite system with higher thermal properties, the main goal of this work was to expand on the encouraging findings from preceding research and apply them to a different material configuration.

Heat conductivity numerical studies hold significance for several reasons. It costs an enormous number of resources to conduct tests to measure heat conductivity since there are the materials, labor, and equipment needed. Using numerical simulations may decrease expenditures by replacing costly trials with a more feasible alternative. Particularly compared to experimental investigations, numerical simulations could potentially be carried out rather quickly, giving researchers more time to investigate a larger range of scenarios and factors. Complex configurations, boundary conditions, and the characteristics of materials can be examined with flexibility using numerical simulations, which might be challenging or unattainable to execute in experimental environments. Scientific progress can be enhanced, and collaboration facilitated by the easily shareable and investigated data that numerical examinations make available to other researchers. Scientists and engineering professionals can optimize designs and forecast the performance of heat exchange systems under numerous circumstances by using established numerical models for predictive purposes. In general, numerical studies provide economical, effective, and versatile tools for investigation and application in engineering, hence supplementing experimental approaches in the study of heat conductivity. The findings we obtained demonstrated that one of the primary variables contributing to the enhanced thermal conductivity of the system made of composites was an increase in copper-chromium thickness. On the other conjunction, an increase in carbon content had the opposite effect, diminishing thermal conductivity. Following a result, we concluded to the conclusion that the material's thickness represented the most significant variable in achieving enhanced thermal conductivity.

Reference

[1] Q. Li, C. Yang, S. Santhanagopalan, K. Smith, J. Lamb, L. A. Steele, and L. Torres-Castro, "Numerical investigation of thermal runaway mitigation through a passive thermal management system", Journal of Power Sources, vol. 429, pp. 80-88, 2019.

[2] Y. H. Kim, D. K. Lee, H. G. Cha, C. W. Kim, Y. C. Kang, and Y. S. Kang, "Preparation and characterization of the antibacterial Cu nanoparticle formed on the surface of SiO2 nanoparticles", The Journal of Physical Chemistry B, vol. 110, pp. 24923-24928, 2006.

[3] L. M. Davis and D. W. Thompson, "Novel and facile approach to the fabrication of metal patterned dielectric substrates", Chemistry of Materials, vol. 19, pp. 2299-2303, 2007.

[4] C. Zweben, "Advances in composite materials for thermal management in electronic packaging", JOM, vol. 50, pp. 47-51, 1998.

[5] P. K. Schelling, L. Shi, and K. E. Goodson, "Managing heat for electronics", Materials Today, vol. 8, pp. 30-35, 2005.

[6] W. Buchgraber, G. Korb, T. Schubert, and B. Kempf, "Carbon fibre reinforced copper matrix composites: Production routes and functional properties", Microstructural Investigation and Analysis, vol. 4, pp. 150-155, 2000.

[7]. S. Berber, Y.-K. Kwon, and D. Tománek, "Unusually High Thermal Conductivity of Carbon Nanotubes", Physical Review Letters, vol. 84, pp. 4613-4616, 2000.

[8]. R. C. Chu, R. E. Simons, M. J. Ellsworth, R. R. Schmidt, and V. Cozzolino, "Review of cooling technologies for computer products", IEEE Transactions on Device and Materials Reliability, vol. 4, pp. 568-585, 2004.

[9] A. Rape, "Copper matrix composites fabricated via field assisted sintering technology for thermal management applications", Ph.D. Thesis, The Pennsylvania State University, 2015.

[10] Y. Sun, L. He, C. Zhang, Q. Meng, B. Liu, K. Gao, M. Wen, and W. Zheng, "Enhanced tensile strength and thermal conductivity in copper diamond composites with B 4 C coating", Scientific Reports, vol. 7, pp. 1-10, 2017.

[11] T. Schubert, W. Zieliński, A. Michalski, T. Weißgärber, and B. Kieback, "Interfacial characterization of Cu/diamond composites prepared by powder metallurgy for heat sink applications", Scripta Materialia, vol. 58, pp. 263- 266, 2008.

[12] D. Zhu, W. Yu, H. Du, L. Chen, Y. Li, and H. Xie, "Thermal conductivity of composite materials containing copper nanowires", Journal of nanomaterials, vol. 2016, pp. 1-6, 2016.

[13] L.-C. Jia, Y.-F. Jin, J.-W. Ren, L.-H. Zhao, D.-X. Yan, and Z.-M. Li, "Highly thermally conductive liquid metal-based composites with superior thermostability for thermal management", Journal of Materials Chemistry C, vol. 9, pp. 2904-2911, 2021.

[14] K. Iqbal, J. J. Sha, Z.-K. Lei, A. Maqsood, and M. Mujahid, "Numerical studies of infiltration dynamics of liquid–copper and silicon/solid– carbon system", JOM, vol. 66, pp. 953-959, 2014.

[15] K. Iqbal, "Numerical studies of infiltration dynamics of liquid-copper and titanium/solid-carbon system", Processing and Properties of Advanced Ceramics and Composites VII: Ceramic Transactions, Volume 252, pp. 157-167, 2015.

[16] K. Woo, D. Kim, J. S. Kim, S. Lim, and J. Moon, "Ink-Jet printing of Cu− Ag-based highly conductive tracks on a transparent substrate", Langmuir, vol. 25, pp. 429-433, 2009.

[17] N. Balachander, I. Seshadri, R. J. Mehta, L. S. Schadler, T. Borca-Tasciuc, P. Keblinski, and G. Ramanath, "Nanowire-filled polymer composites with ultrahigh thermal conductivity", Applied Physics Letters, vol. 102, p. 093117, 2013.

[18] S. Kumar, A. Kumar, R. Devi, A. Shukla, and A. Gupta, "Capillary infiltration studies of liquids into 3D-stitched C–C preforms: Part B: Kinetics of silicon infiltration", Journal of the European Ceramic Society, vol. 29, pp. 2651-2657, 2009.

[19] S. Wu, T. Yan, Z. Kuai, and W. Pan, "Thermal conductivity enhancement on phase change materials for thermal energy storage: A review", Energy Storage Materials, vol. 25, pp. 251-295, 2020.

[20] Koltsova, T., Bobrynina, E., Vozniakovskii, A., Larionova, T., & Klimova-Korsmik, O. "Thermal Conductivity of Composite Materials Copper-Fullerene Soot". Materials, 15(4), 1415, 2022.

[21] Zuo, Q., Wang, W., Gu, M. S., Fang, H. J., Ma, L., Wang, P., ... & Zhang, Y. J. "Thermal conductivity of the Diamond-Cu composites with chromium addition". Advanced Materials Research, 311, 287-292, 2011.

[22] Chu, K., Liu, Z., Jia, C., Chen, H., Liang, X., Gao, W., ... & Guo, H. "Thermal conductivity of SPS consolidated Cu/diamond composites with Cr-coated diamond particles". Journal of Alloys and Compounds, 490(1-2), 453-458, 2010.

[22] Zhang, X., Guo, X., Song, K., Wang, X., Feng, J., Li, S., & Lin, H." Simulation and verification of thermal conductivity of CuCr30 contact material based on morphological changes of Cr particles". Materials Today Communications, 26, 102153, 2021.

[23] Zhao, D., Zha, S., & Liu, D. "Influence of sputtering and electroless plating of Cr/Cu dual-layer structure on thermal conductivity of diamond/copper composites". Diamond and Related Materials, 115, 108296, 2021.

[24] Liu, X., Sun, F., Wang, L., Wu, Z., Wang, X., Wang, J., ... & Zhang, H. "The role of Cr interlayer in determining interfacial thermal conductance between Cu and diamond". Applied Surface Science, 515, 146046, 2020.

[25] Minghe, C., Hongzhao, L., Changrui, W., Ning, W., Zhiyou, L., & Lina, T. “Progress in heat conduction of diamond/Cu composites with high thermal conductivity”. Rare Metal Materials and Engineering, 49(12), 2020.

[26] Dong, X., & Shin, Y. C. “Multi-scale modeling of thermal conductivity of SiC-reinforced aluminum metal matrix composite”. Journal of Composite Materials, 51(28), 3941-3953, 2017.

[27] Liao, Q., Wei, W., Zuo, H., Li, X., Yang, Z., Xiao, S., & Wu, G. “Interfacial bonding enhancement and properties improvement of carbon/copper composites based on nickel doping”. Composite interfaces, 28(6), 637-649, 2021.

[28] Ali, A., & Iqbal, K.” Numerical study on a heat transfer model in the solid-carbon/liquid-copper system”. Mehran University Research Journal of Engineering & Technology, 41(3), 185-190, 2022.

[29] T. Schubert, A. Brendel, K. Schmid, T. Koeck, W. Zieliński, T. Weißgärber, and B. Kieback, "Interfacial design of Cu/SiC composites prepared by powder metallurgy for heat sink applications", Composites part A: Applied science and Manufacturing, vol. 38, pp. 2398-2403, 2007.

[30] K. Chu, Z. Liu, C. Jia, H. Chen, X. Liang, W. Gao, W. Tian, and H. Guo, "Thermal conductivity of SPS consolidated Cu/diamond composites with Crcoated diamond particles", Journal of Alloys and Compounds, vol. 490, pp. 453-458, 2010.