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Research Trends in the Heat Transfer Simulation of Al_2O_3/AlN Granular Composites for Thermal Interface Materials

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Abstract: Heat transfer simulation in granular Al_2O_3/AlN composites has become an increasingly relevant topic in the development of thermal interface materials (TIMs) for high-performance electronic systems. This study conducted a bibliometric analysis of 1,169 articles from the Scopus database published between 2015 and 2025 to identify research trends, frequently occurring keywords, geographic contributions, author and institutional impacts, and to outline future research opportunities in the development of TIMs based on Al_2O_3/AlN. The analysis was performed using RStudio, VOSviewer, and Excel, identifying five main thematic clusters: (1) AI and Neuroimaging for Brain Diseases; (2) TIM Applications and Thermal Optimization; (3) Molecular Simulation and Interface Properties; (4) AI and Brain Functional Connectivity; (5) Numerical Simulation of Material Thermal Properties and (6) Materials & Thermal Contact Resistance. The primary research focus includes numerical modeling of thermal conductivity, characterization of Al_2O_3 and AlN materials, and their initial applications in electronic cooling devices. While the scope remains limited at present, the annual growth in publications suggests that interest in this topic is likely to increase soon. This study provides an important initial overview of the research landscape. It opens up possibilities for future exploration, including the integration of multiscale approaches and enhanced experimental validation in heat transfer simulations involving granular composites.

Keywords: Bibliometric analysis, Thermal interface materials, Al_2O_3/AlN composites, Heat transfer simulation, Advanced computational methods

Introduction

Effective heat management is crucial in modern electronic devices, including smartphones, CPUs, and electric vehicles. As devices become smaller in size and more power-dense, heat accumulation becomes a significant issue that can reduce performance and lead to component failure if the temperature exceeds safe limits (Ghadim et al., 2025). Uneven temperature distribution and the appearance of hotspots accelerate component degradation (Z. He et al., 2020). To address these issues, various strategies, including micro heat sinks, Phase Change Materials (PCMs), and innovative heat sink designs, have been developed to enhance thermal conductivity (Bianco et al., 2022). PCMs can stabilize the temperature but still face challenges in terms of long-term durability and efficiency (Liu et al., 2022). Hybrid systems that combine heat management and recovery are also being developed for miniaturized and autonomous devices (Wang et al., 2020).

One important component in heat management is Thermal Interface Materials (TIMs), which function to reduce the thermal resistance between two solid surfaces, such as between a chip and a heat sink, thus enabling more efficient heat transfer (Razeeb et al., 2018). Thermal resistance at the interface is often a significant obstacle due to microscopic air gaps that act as insulators (Chung, 2022). To overcome this, TIMs such as thermal paste, liquid metal, and graphene-based materials have been developed to fill these gaps and improve thermal contact (Sudhindra et al., 2021). Recent advances involve technologies such as self-assembled monolayers (SAMs) and graphene-coated copper nanowires, which significantly reduce thermal resistance (He et al., 2024). In addition, the development of phase change-based TIMs and flexible materials opens up new possibilities for future electronic devices (Jing et al., 2023). The interaction between the filler and the polymer matrix plays a crucial role in enhancing thermal conductivity (Haoqi et al., 2020).

However, challenges persist due to surface unevenness, material property differences, and a limited contact area between solid components (Liang et al., 2025). These imperfections result in high thermal resistance, impeding heat flow (Dai et al., 2022). Interface structure engineering efforts, such as the use of nanopillars and nanocones, show potential in increasing the contact area and thermal conductivity (Lee et al., 2016). Other materials, such as graphene-based interfaces and liquid metals, can also significantly reduce thermal resistance (Wang et al., 2023). Advanced approaches such as the application of nano-mass graded interfaces are also effective in reducing phonon reflection and improving heat transmission between different materials (Zhou et al., 2016). Further development is still needed to balance thermal conductivity, mechanical stability, and chemical compatibility between materials (Zeng et al., 2024). Therefore, innovative solutions that combine structural engineering, material selection, and surface modification are crucial for overcoming thermal barriers and enhancing heat transfer efficiency in modern electronic devices (Zhou et al., 2016).

Al_2O_3/AlN granular composites offer significant synergies for thermal interface materials thanks to their unique physical and chemical properties. Al_2O_3 is renowned for its hardness and corrosion resistance, while AlN excels in thermal conductivity, making it a compelling option for applications that require strength and effective heat management (Wang et al., 2021). This material combination has been investigated for various applications, including electronic components and the automotive industry (Rosadi, 2024). Research shows that AlN enhances the thermal properties of alumina-based composites, where AlN not only serves as a filler but also improves the overall thermal performance (Wang et al., 2021). Additionally, methods such as electrodeposition have been investigated to create cellular structures within these composites, thereby enhancing their thermal and mechanical properties (Maulida, 2024). These innovations are particularly significant in industries where material reliability is crucial for optimal performance, such as in electronics and automotive applications (Wang et al., 2021).

The importance of this research lies in enhancing the practical application of granular composites in heat dissipation, thereby extending the life of components (Wang et al., 2021). As materials technology advances, further research is necessary to explore the potential applications of these composites in the future (Hadi et al., 2022). Numerical simulations offer an advantage in predicting thermal interactions at the microscopic level, which cannot be directly observed. For example, Huang et al. employed the discrete element method (DEM) to investigate the impact of temperature on the behavior of granular materials (Huang et al., 2023). This research helps to understand the relationship between thermal and mechanical interactions, which is crucial in developing efficient heat transfer models for composites such as Al_2O_3/AlN.

Method

Research Design and Data Collection Procedures

This study conducted a descriptive bibliometric analysis to assess the landscape of scientific publications on science literacy from 2015 to 2025. Bibliometric analysis is widely recognized as a reliable approach to reviewing vast scientific literature. It allows researchers to trace the developmental trajectory of a particular discipline and identify emerging trends (Donthu et al., 2021). This approach enables researchers and readers to gain a comprehensive understanding of the research themes explored over time, supported by statistical assessments of academic contributions (Rejeb et al., 2023). Additionally, bibliometric techniques are effective for mapping the intellectual structure of a research field and identifying emerging areas of research. Through performance analysis and scholarly mapping, bibliometrics enable a detailed examination of publication sources, document types, citation patterns, and keyword dynamics (Lethulur, 2024). Bibliometric analysis follows a rigorous multi-stage screening protocol to ensure relevance, scientific rigor, and thematic alignment of the literature (Aria & Cuccurullo, 2017; Donthu et al., 2021; Kusharyadi et al., 2023). This process aligns with the established bibliometric methodology recommended by Singh et al. (2022), which consists of database search, scientific screening, language screening, and subject screening. In stage 1, we conducted a database search. An initial search was conducted in the Scopus database using the keywords "Thermal material interface" or TIM and "simulation" or "modeling" or "computational" or "numerical" from 2015 to 2025. This resulted in the identification of 1,341 documents. The use of Scopus was justified due to its comprehensive coverage of peer-reviewed publications and its standard utilization in bibliometric studies (Paul et al., 2021). In Stage 2, we conducted scientific screening to ensure academic validity, retaining only journal articles and conference proceedings that met the criteria. This stage excluded 96 documents, such as book chapters, editorials, and nonpeer-reviewed items, resulting in 1,245 records. This step aligns with the recommendations of Aria & Cuccurullo (2017), who emphasize the exclusion of grey literature to enhance the scientific credibility of bibliometric datasets. In stage 3, we performed Language Filtering. Next, language filtering was applied to retain only English publications. Out of 1,245 documents, 1,205 met this criterion. This practice ensures consistency in analysis and interpretation, as English remains the dominant language in scientific discourse (Singh et al., 2022). Finally, in stage 4, we performed subject filtering. In the last step, documents were screened for relevance to the subject areas of Engineering, Materials Science, Physics and Astronomy, Computer Science, and Chemical Engineering. Twenty irrelevant articles were excluded, resulting in 604 articles suitable for bibliometric analysis. The subject area refinement step is crucial for maintaining thematic consistency and ensuring the focus of the analysis remains intact (Aria & Cuccurullo, 2017). This structured screening approach ensures the validity and reliability of the dataset used for bibliometric mapping, in line with best practices for systematic reviews and scientific mapping studies (Hajjaji et al., 2021). The sequence of the screening process is visually represented in the flowchart below, which illustrates each stage, from initial identification to final inclusion of documents for analysis.

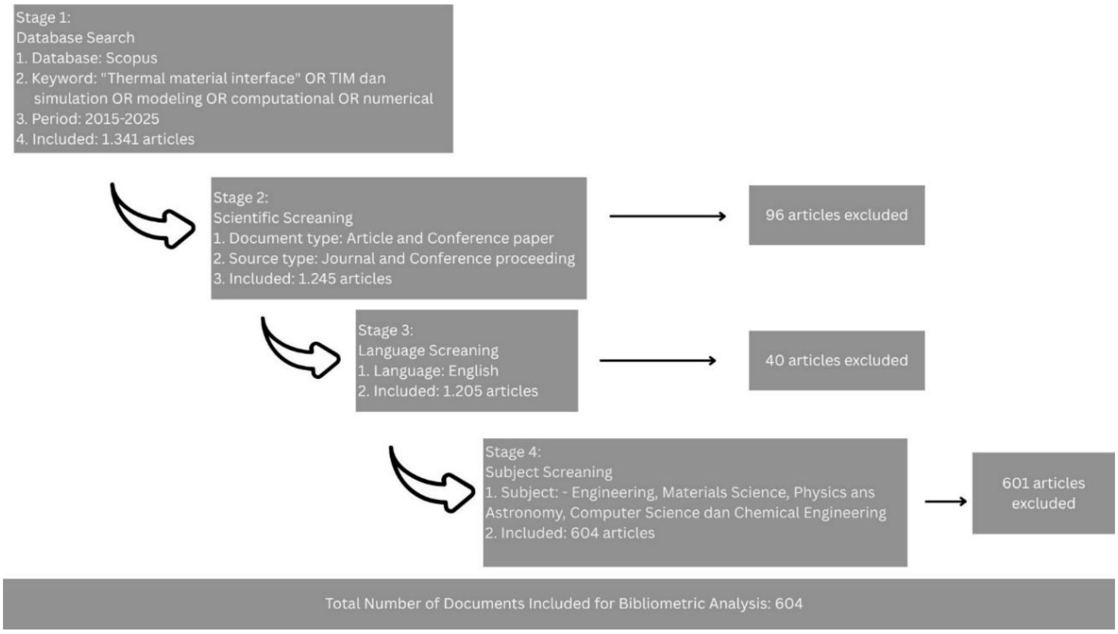

Figure 1. Research design and data collection procedure

Data Analysis Methods, Validity, and Reliability

This study used VOSviewer version 1.6.20 to perform dynamic and structural visualization of the dataset related to Heat Transfer Simulation of Al_2O_3/Aln Granular Composites for Thermal Interface Materials, following established bibliometric procedures (Dönmez, 2024). Data were retrieved from the Scopus database, covering the period 2015 to 2025, and exported in CSV (Comma-Separated Values) format. The CSV format was imported into VOSviewer to build co-authorship networks, identify keyword co-occurrences, and perform citation mapping. Simultaneously, the duplicate CSV files were processed using Biblioshiny, a web-based interface of the R package Bibliometrix, to calculate bibliometric indicators such as h-index, g-index, total citations, and to explore thematic evolution and conceptual structure (Aria & Cuccurullo, 2017). Furthermore, Microsoft Excel was used not only to visualize the global distribution of publication output in different regions on the world map, but also to improve the clarity and readability of the resulting visualizations for better interpretation and presentation.

To strengthen the credibility and transparency of the research process, this study provides comprehensive details of each methodological stage. These details include the exact date of data extraction (June 16, 2025), the syntax of the search string used in the TITLE-ABS-KEY field (i.e., "Thermal material interface" OR TIM AND simulation OR modeling OR computational OR numerical), the inclusion and exclusion criteria, and the screening flow clearly outlined in the attached process diagram. The analysis adhered to methodological rigor by documenting the screening steps in four stages: database search, scientific screening, language screening, and subject area relevance, resulting in a final dataset of 604 documents eligible for bibliometric analysis.

Most importantly, this study does not present interpretative commentary on the findings, thus ensuring objectivity and analytical precision. Ethical approval was not required, as this dataset contains only open-access metadata sourced from the Scopus database. The overall methodological framework is aligned with recommended standards for systematic mapping and bibliometric reviews, thus ensuring the validity and reliability of the results for further scientific use.

Results and Discussion

The following will explain the research trends in thermal interface materials, the countries with the most significant contributions to Thermal interface materials research, VOS Viewer Visualization Analysis, and the novelty and focus of Thermal interface materials research.

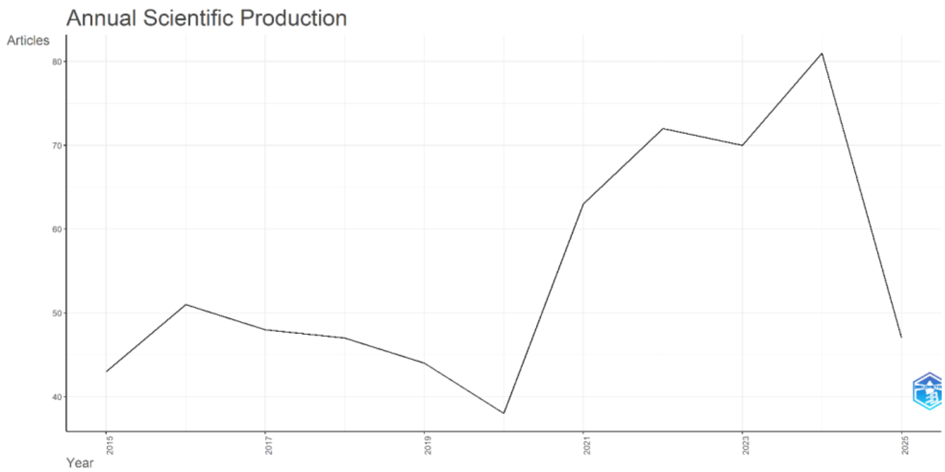

Figure 2. Publication trends

Figure 2 illustrates the trend of annual scientific production, highlighting the dynamics of research development in the topic over the period from 2015 to 2025. At the beginning of the period (2015-2020), the number of publications remained relatively stagnant, with a slight decrease, and reached its lowest point in 2020, indicating that this topic had not yet garnered widespread attention in the scientific community. However, starting in 2021, there was a significant spike in the number of publications, reaching its peak in 2023 with a total of 81 articles, reflecting the increasing urgency and relevance of this research as the need for thermal interface materials for high-power electronic systems grows. This phenomenon can also be attributed to advances in thermal simulation technology as well as increased cross-disciplinary collaboration. However, a downward trend is again seen from 2024 to 2025, which could be due to several factors, such as a shift in research focus, limited funding, or data that has not been fully accumulated for the last year. Overall, this pattern reflects a typical evolutive development in a new research field that is growing and consolidating.

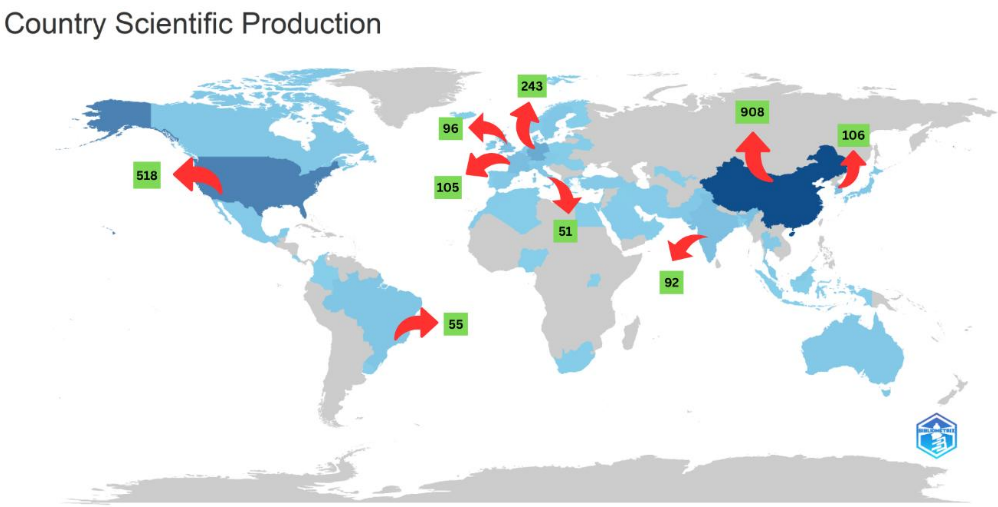

Figure 3. Geographic distribution

Based on the geographical distribution of scientific publications in Figure 3, China holds the leading position with a total of 908 publications, demonstrating a strong dominance in related research, which reflects the country's aggressive national policy in supporting the research and development of advanced materials for thermal technology. The United States ranked second, with 518 publications, indicating consistent contributions from both academic institutions and industry in the development of thermal simulation approaches. Germany, as a leader in technology research in Europe, recorded 243 publications, followed by South Korea (106) and France (105), indicating active involvement from countries with strong traditions in materials engineering and applied physics. The UK (96), India (92), Brazil (55), and Italy (51) also contributed significantly, showing that research on this topic is global and involves cross-regional cooperation. This pattern reflects not only national scientific capacity but also the strategic priorities of these countries in developing efficient thermal solutions for future electronic systems.

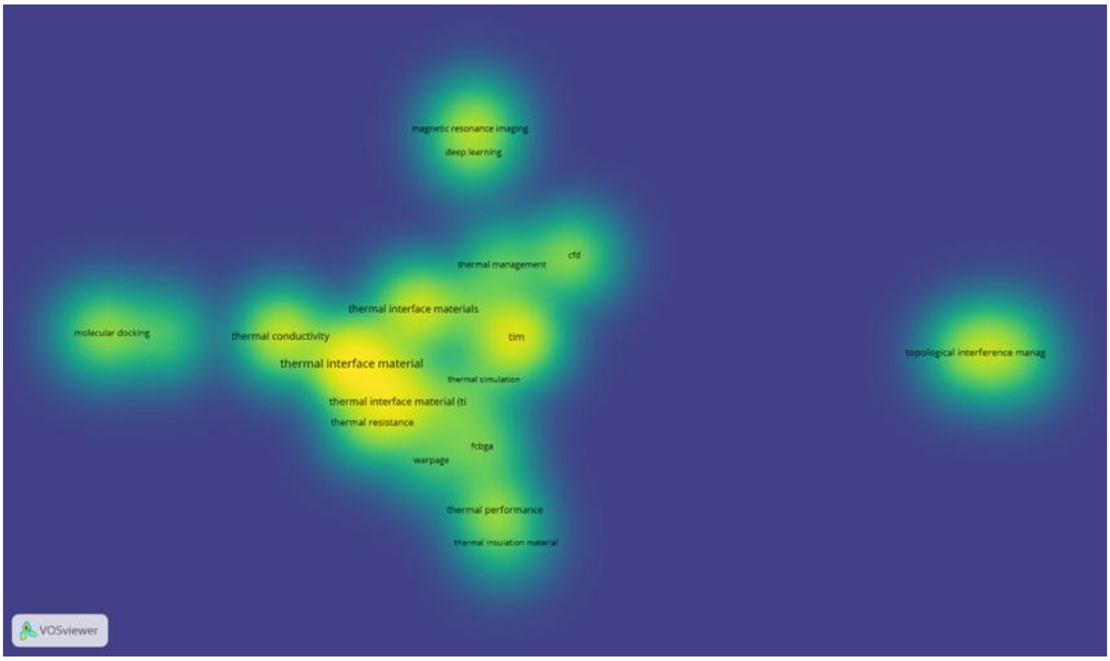

Figure 4. Density overlay

The density overlay visualization generated using VOSviewer shows the density of keyword distribution in the literature related to thermal interface materials (TIM) research. Areas in bright yellow represent a high concentration of frequently used keywords, such as thermal interface materials, thermal conductivity, thermal resistance, and thermal simulation. This indicates that the primary focus of research in this field remains centered on enhancing heat transfer efficiency and characterizing the thermal properties of materials. On the other hand, several keywords appear in lower density areas, such as deep learning, magnetic resonance imaging, and molecular docking. Although the frequency of occurrence is still limited, these keywords indicate an initial trend towards interdisciplinary approaches, such as the integration of artificial intelligence and molecular techniques in thermal performance modeling or optimization. The presence of terms such as CFD (computational fluid dynamics) and thermal management shows the interconnectedness of TIM research with systems and numerical engineering approaches. Interestingly, the appearance of terms such as topological interference management, although likely an incomplete entry, could signal new directions that could potentially be developed, such as exploring the topological properties of materials in the context of thermal management. Overall, this visualization not only confirms the dominant themes in TIM research but also reveals potential new research developments at the interdisciplinary nexus between materials technology, artificial intelligence, and advanced computational simulation that are still relatively open for exploration.

Figure 5 presents the bibliometric analysis conducted on publications related to thermal interface materials (TIM) that utilize simulation and computational approaches, resulting in a total of 26 keywords that form six main thematic clusters. This visualization and mapping were carried out using VOSviewer software to identify interrelationships between concepts and group interconnected research trends. Each cluster reflects a particular research focus that complements each other in the development and utilization of TIM, both from theoretical, experimental, and applicative aspects. The following descriptions explain the main themes and scientific context of each identified cluster.

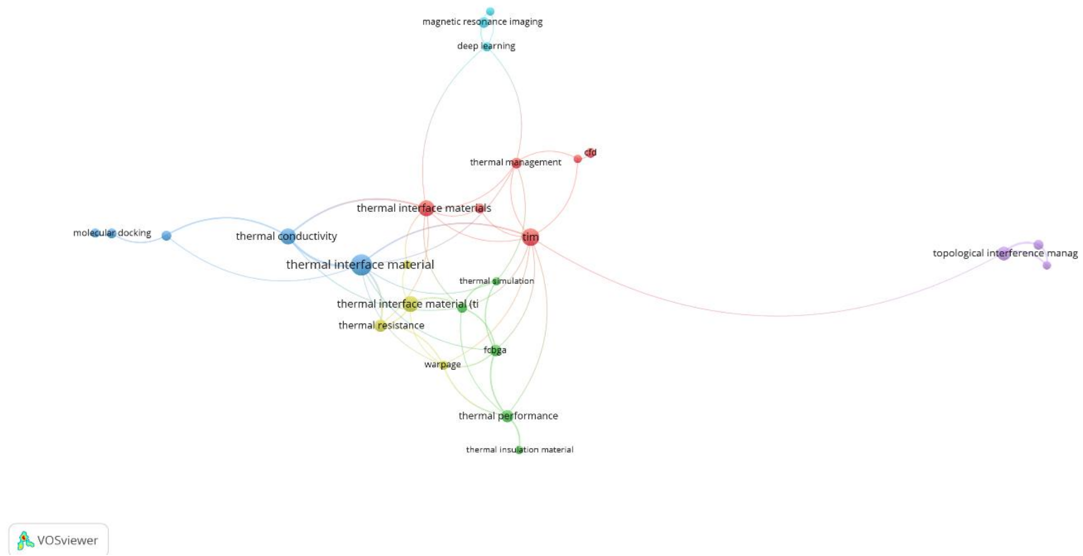

Figure 5. Network visualization

Cluster 1 is the dominant center in the visualization map, as it encompasses a range of basic to advanced applications of thermal interface materials (TIMs). Terms such as computational fluid dynamics (CFD), simulation, and thermal management indicate that many research trends focus on numerical modeling to optimize heat management in electronic systems. On the other hand, the presence of the keyword reliability signifies that the continued functioning of the electronic system is highly dependent on the thermal efficiency provided by the TIM. The utilization of simulation becomes crucial for designing and evaluating the thermal performance before experimental implementation is undertaken. This cluster highlights the significance of computational approaches in addressing real-world problems in thermal design, particularly in high-power systems such as processors, batteries, and electric vehicles. Cluster 2 encompasses the study of electronic package architecture and passive components that enhance thermal performance, including heat sinks and insulation materials. FCBGA (flip-chip ball grid array) is a type of microelectronic package that is complex and highly sensitive to heat distribution. Studies in this cluster typically evaluate the performance of these components using thermal simulation to enhance heat release efficiency and reduce the device's working temperature. Research in this cluster focuses on developing efficient cooling systems through physical design and the selection of thermal insulating materials. Cluster 3 indicates molecular simulation-based approaches to understand the fundamental properties of TIM materials. Methods such as molecular dynamics simulation and molecular docking are employed to analyze interactions between atoms, bonding energies, and heat transfer mechanisms at the nanoscale. The primary focus is to maximize the thermal conductivity of the material through a deep understanding of its microscopic structure. This cluster plays an important role in the design of nanotechnology-based materials and composites, which can exhibit high thermal performance through atomic structure and interfacial engineering. Cluster 4 is concerned with the issues of thermal deformation (warpage) and thermal resistance in structures using TIM. Thermal analysis is performed to assess the mechanical integrity of components during heating and cooling processes, especially in multi-layer structures and polymeric materials. Thermal resistance is a crucial indicator in evaluating the efficiency of heat transfer between layers. Demonstrates the relevance of integrating thermal analysis with structural aspects, so that material design can consider not only conductivity, but also shape stability and thermomechanical durability. Cluster 5 is more theoretical and describes mathematical approaches in signal or heat management through topological structures. Concepts such as low-rank matrix completion and interference alignment demonstrate the application of linear algebra and numerical optimization techniques, particularly in the context of thermal communication or multi-channel systems. This reflects a new trend in combining high computational methods with the design of physical structures, leading to the integration of disciplines such as information theory and topological engineering for managing heat or signals in complex systems. At the same time, cluster 6 represents a recent trend in the literature, namely the use of machine learning and deep learning to analyze and predict material performance based on numerical data or images. The integration with magnetic resonance imaging (MRI) technology demonstrates the potential for using non-destructive imaging to detect the internal thermal properties of TIM materials. Serving as a bridge between materials science and data science, it opens up opportunities to explore AI-based predictive methods for material design optimization without the need for extensive physical experiments.

cfd, reliability, simulation, thermal interface materials, thermal management, tim	**fcbga, heat sink, thermal insulation material, thermal performance, thermal simulation**	**molecular docking, molecular dynamics, molecular dynamics simulation, thermal conductivity, thermal interface material**	**thermal analysis, thermal interface material (ti), thermal resistance, warpage**	**interference alignment, low-rank matrix completion, topological interference management**	**deep learning, machine learning, magnetic resonance imaging**

Figure 6. Categorization of keywords

The six identified clusters show that the study of thermal interface materials (TIMs) is highly multidisciplinary, spanning materials physics, electrical engineering, numerical simulation, artificial intelligence, and even topological approaches. The primary trend is towards integrating predictive models with the structural understanding of materials to achieve maximum thermal performance in modern electronic devices.

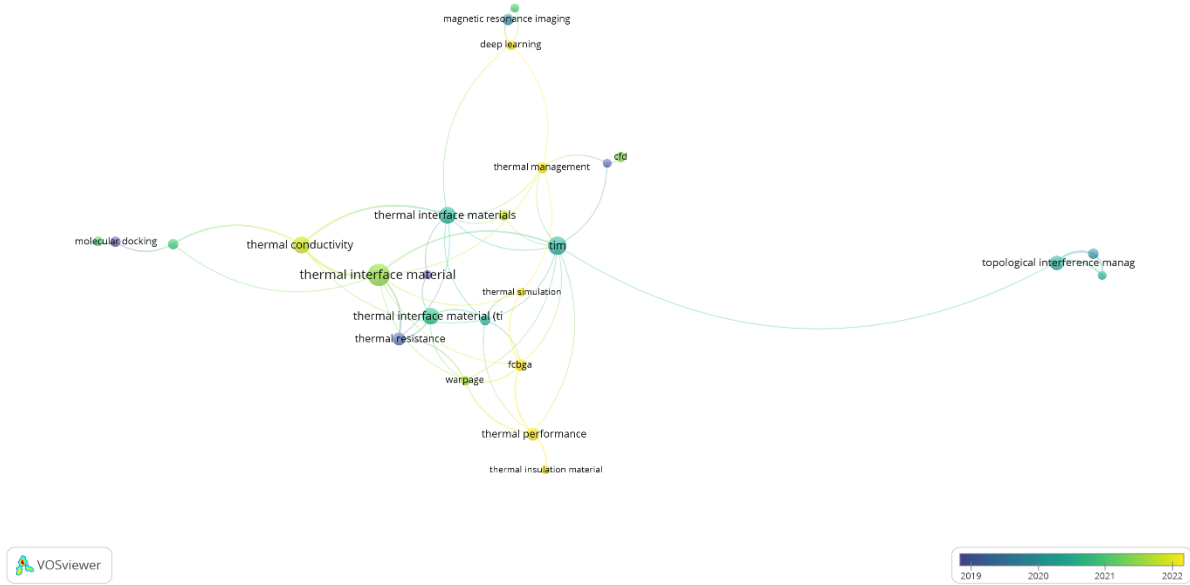

Figure 7. Overlay visualization

The overlay visualization of the bibliometric analysis generated through VOSviewer illustrates the temporal dynamics of keyword occurrence in the literature related to thermal interface materials (TIM) research. This map employs a spectral color gradation, ranging from purple (representing the average occurrence around 2019) to yellow (indicating the average occurrence near 2022), which illustrates the progression of time for the topics explored. Primary keywords such as thermal interface materials, thermal resistance, and thermal simulation appear in bluish-purple, indicating that early research in this field focused heavily on fundamental aspects of materials, including thermal resistance and numerical simulation approaches to evaluate thermal performance. Over time, there has been a shift in focus marked by the emergence of terms such as thermal conductivity, thermal performance, and thermal insulation of materials, ranging from greenish yellow to bright yellow. This suggests that recent studies have begun to focus on enhancing the efficiency and specific capabilities of TIM materials in practical applications, particularly in high-power electronic systems.

Furthermore, the emergence of buzzwords such as deep learning, magnetic resonance imaging, and molecular docking, accompanied by bright colors, signifies a new trend towards the integration of interdisciplinary approaches. These approaches include the application of artificial intelligence for materials modeling and optimization, as well as molecular imaging and simulation techniques, to more accurately explore the microstructure of materials. Meanwhile, terms such as topological interference management, while still low in frequency and on the periphery of the network, indicate the potential of emerging new directions in the context of manipulating the topological properties of materials for more efficient heat management. The appearance of such terms in light green indicates that the topic is starting to attract attention in the middle period (around 2020-2021). It has the potential to grow into a more established research area. Therefore, this visualization not only reveals the conceptual evolution in TIM research but also maps the emergence of new areas that could form the basis for further novel, cutting-edge, and multidisciplinary research.

Discussion

The bibliometric analysis conducted in this study successfully revealed the intellectual structure and direction of research development in the field of thermal interface materials (TIM), particularly in the context of heat transfer simulation in Al_2O_3/AlN granular composites. Through keyword co-occurrence mapping with VOSviewer, six thematic clusters are identified, revealing the diversity of research approaches and focuses. These findings not only illustrate the current landscape of literature but also provide insights into potential pathways for further scientific exploration.

Cluster 1 is the focal point of the bibliometric network as it covers key terms such as thermal interface materials, simulation, thermal management, CFD, and reliability. The main focus of research in this cluster is on numerical approaches, particularly computational fluid dynamics (CFD), to analyze and optimize heat transfer between components in high-power electronic systems. Numerical models offer an efficient and cost-effective alternative to experimental approaches, enabling the evaluation of various geometry configurations and working conditions prior to fabrication. The use of simulation is also relevant in assessing long-term reliability, as modern electronic systems must be able to withstand extreme thermal fluctuation conditions. As such, this cluster provides a methodological foundation for the design of precise and predictive Al_2O_3/AlN-based TIM materials. Unlike Cluster 1, which emphasizes computational approaches, Cluster 2 focuses on hardware-level integration, covering keywords such as FCBGA, heat sinks, thermal insulation materials, thermal performance, and thermal simulations. FCBGA is a temperature-sensitive chip packaging technology, and studies in this cluster aim to evaluate the effectiveness of passive and active cooling systems, such as heat sinks, in maintaining the thermal stability of devices. A simulative approach to electronic package configuration is crucial for reducing the hotspot phenomenon and maintaining temperature homogeneity across component surfaces. In addition, the presence of insulation materials emphasizes attention to the energetic efficiency of the system and the reduction of unwanted heat losses. The primary contribution of this cluster is the enhancement of the connection between the physical design of components and the overall thermal performance of the system, particularly in micro- and nanoscale applications. Cluster 3 is about molecular simulation and material structure engineering. This cluster covers advanced topics at the atomistic level, including molecular dynamics, molecular docking, and thermal conductivity. Molecular simulation enables an in-depth understanding of the heat transfer mechanisms that occur within and between granular grains, as well as the phonon interactions between interfaces. This approach is particularly critical in composite systems, such as Al_2O_3/AlN, where the bonding between particles, particle size, and matrix structure have a significant influence on thermal conductivity. With molecular docking methods, researchers can assess how the orientation and distribution of filler materials within the matrix impact the heat conduction pathway. This understanding opens up opportunities for precise interfacial engineering at the nanoscale, with the hope of improving thermal boundary conductance and reducing thermal resistance. This cluster strengthens the connection between statistical physics, phonon theory, and materials science. Cluster 4 focuses more on structural evaluation and thermal warpage analysis, with a particular emphasis on thermal resistance, thermal analysis, and warpage. Structural issues, such as deformation due to thermal loads (warpage) and the mechanical stability of TIMs, are of major concern. In multi-layer systems, such as those using Al_2O_3/AlN granular composites, a mismatch in the coefficient of thermal expansion (CTE) between layers can generate residual stresses that lead to delamination, cracking, or deformation. The analysis in this cluster examines the impact of geometric and thermomechanical factors on thermal performance, as well as their influence on the device's service life and structural integrity. As such, this cluster highlights the importance of combining thermal performance and mechanical stability as two inseparable requirements in the development of reliable and durable TIMs. Despite its relatively small size and frequency, Cluster 5, which consists of keywords such as topological interference management, interference alignment, and low-rank matrix completion, represents innovative mathematical and topological approaches. These concepts are commonly used in signal processing and communication network optimization, but their adaptation in the domains of heat management and material structure design is beginning to show potential. For example, low-rank optimization approaches can be employed to design material configurations with optimal microstructures, thereby enhancing heat conduction pathways. The technique is also relevant in data-driven material discovery, where mapping material properties based on non-linear relationships and topological structures can accelerate the development of new generation TIM materials. Although currently exploratory, this direction could serve as a stepping stone towards integrating differential geometry, statistical mechanics, and high computing technology in functional material design. The last cluster shows a new trend in the integration of machine learning (ML) and deep learning (DL) in TIM studies. The presence of buzzwords such as magnetic resonance imaging (MRI) indicates that non-destructive imaging methods are now being adopted to evaluate the thermal distribution and internal integrity of TIM materials in real-time. ML-based approaches enable more efficient and accurate processing of simulation or image data and pave the way towards AI-based predictive systems for designing and testing materials without the need for repeated physical experiments. In the context of granular composite materials, ML models can be trained to recognize microstructure patterns that correlate strongly with thermal conductivity, enabling data-driven design optimization. This cluster reflects the methodological transformation in materials research, where material informatics is becoming an increasingly integrated domain with materials physics and engineering.

Overall, the six identified clusters indicate a complex and multidimensional direction of development in Al_2O_3/AlN granular composite-based TIM research. Research in this area is no longer limited to conventional experiments or macroscopic measurements, but has evolved to include multiscale simulations, AI integration, topological optimization, and molecular approaches. The complexity of thermal problems in modern electronic systems drives the need for holistic and adaptive solutions. As such, the results of this study provide an important foundation for understanding the current knowledge structure and identifying relevant research gaps for further exploration.

Conclusion

This study has uncovered a comprehensive scientific landscape of thermal interface materials (TIM) research trends, particularly in the context of heat transfer simulation in Al_2O_3/AlN granular composites, through a bibliometric approach of 604 publications from the Scopus database during the period 2015-2025. Using VOSviewer and keyword co-occurrence analysis, six thematic clusters were identified, each reflecting different research directions and approaches, ranging from numerical simulation and hardware design to molecular modeling, structural evaluation, and the integration of artificial intelligence and topological methods.

These results show that research on TIM is undergoing significant multidisciplinary development. The dominance of simulation-based and molecular approaches signifies the importance of an in-depth understanding of heat transfer mechanisms at both micro and macro scales. Meanwhile, the emergence of artificial intelligence integration and advanced characterization techniques signals the transition towards a new paradigm in data-driven material design.

Overall, these findings provide an important strategic overview for researchers, practitioners, and technology developers to understand the direction of TIM research development and find gaps that can be further explored. The combination of material structure engineering, multiscale simulation, and the utilization of digital technologies such as AI is a key driver for the development of future TIMs that are more efficient, reliable, and applicable to high-power electronic systems.

Recommendations

Based on the results and discussions in this study, a number of strategic recommendations can be proposed to encourage the development of research and applications of thermal interface materials (TIM) based on Al_2O_3/AlN granular composites in a more progressive and applicable direction:

1. Strengthening Multiscale and Multidisciplinary Research

Stronger integration between molecular simulation, macroscopic numerical computation, and experimental validation is needed. This multiscale approach will enhance the accuracy of models in predicting the thermal and mechanical properties of granular composites, while also reducing the gap between simulation and practical implementation.

2. Data-Driven Predictive Model Development and Artificial Intelligence

The application of machine learning and deep learning to develop predictive models for thermal conductivity and mechanical stability of TIM materials remains largely unexplored. Model training based on simulation datasets and experimental results can efficiently and economically accelerate the design and selection process of new materials.

3. Exploration of Interface Structure Engineering

Expanding the study of complex interface structures, such as graded interfaces, nanopillar arrays, or interfaces with topological modifications (e.g., through micro-molding or lithography techniques), will enrich the options for increasing thermal boundary conductance. This is especially important for TIM integration in high-power semiconductor systems.

4. Further Experimental Validation under Real-World Conditions

Future research should extend the experimental test scenarios to TIM in real-world environments, such as those with temperature fluctuations, cyclic stress, or exposure to electromagnetic fields. This validation is crucial for bridging the gap between idealized performance in simulation and actual stability in long-term applications.

5. Facilitate International and Interdisciplinary Collaboration

Given the increasingly complex and fragmented trend in TIM research, cross-country and interdisciplinary collaborations among materials physicists, mechanical engineers, computer experts, and the manufacturing industry are highly recommended to accelerate the adoption of innovative and industry-appropriate TIM technologies.

6. Improved Access and Standardization of Material Simulation Data

The development of an open database containing thermal simulation results and characterization of TIM composites, encompassing both microscopic and macroscopic parameters, is necessary. Standardization of data formats will facilitate interoperability across simulation platforms and strengthen research reproducibility.

These recommendations are expected to serve as a practical and conceptual guide for the scientific community in directing thermal interface materials research toward results that are more effective, innovative, and have a broad impact on the development of future electronic technology.

Scientific Ethics Declaration

* The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Conflict of Interest

* The authors declare that they have no conflicts of interest

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