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Thermal Interface Materials and Two-Dimensional Nanomaterials for High-Density Data Center Thermal Management

Yurucheng Zhang

School of Communication and Information Engineering, Shanghai University, Shanghai, China
2502621075@qq.com

Abstract. The proliferation of high-performance computing (HPC) and artificial intelligence (AI) workloads has given rise to unprecedented power densities in data center hardware, positioning thermal management as a critical bottleneck constraining system performance, long-term reliability, and energy efficiency. This paper clarifies the role of advanced thermal interface materials (TIMs) in addressing thermal management challenges in high-density data centers, with a particular focus on nanostructured systems and emerging two-dimensional materials such as graphene and hexagonal boron nitride (h-BN). Accordingly, this study analyzes the physical origins of thermal bottlenecks, including interfacial thermal resistance (ITR) and localized hotspots, and assesses the development and performance of advanced TIMs. And it further compares conventional particle-filled composites with nanostructured materials, thus highlighting the interplay among material properties, interfacial heat transfer mechanisms, and practical implementation challenges. Results show that two-dimensional nanomaterials provide promising solutions through enhanced thermal transport and interface engineering, although limitations associated with scalability, integration complexity, and phonon mismatch remain significant barriers for real-world deployment.

Keywords: data center, thermal management, thermal interface material, 2D nanomaterial, graphene, hexagonal boron nitride

1. Introduction

Driven by cloud computing, big data analytics and large-scale artificial intelligence models, global demand for computational throughput has grown at an unprecedented rate over the past decade. As the key infrastructure for the digital economy, data centers are adopting higher-density computing hardware to meet growing demands, driving increased power density at both chip and rack levels. According to recent reports, the average surface power density of state-of-the-art HPC processors has exceeded 100 W/cm^{2,} while the peak heat flux of on-die hotspots has reached over 2000 W/cm^2 in publicly reported cases [1]. Furthermore, cooling systems account for 30%–40% of total energy consumption in conventional data centers, making thermal efficiency a key component of sustainable development [2]. Traditional thermal management paradigms, designed for low-density

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systems, have become a major constraint on system performance, reliability and energy efficiency. In this context, advanced thermal interface materials (TIMs) based on low-dimensional nanomaterials have emerged as promising solutions for overcoming the thermal limitations of next-generation computing systems. This paper reviews advances in thermal management materials for high-density data centers, focusing on TIM evolution and representative 2D nanomaterials, including graphene and hexagonal boron nitride (h-BN). The mechanisms of thermal bottlenecks in electronic packaging are examined, followed by analyses of conventional, structured, and 2D material-based TIMs in terms of thermal properties, interfacial transport, and implementation challenges. Commercial validation cases and future research directions beyond material optimization are further discussed to provide insights into the development of thermal management technologies for next-generation high-density data centers.

2. Thermal challenges and material requirements for high-density computing

The heat dissipation inefficiency of modern microelectronic systems originates mainly from two interrelated physical phenomena: interfacial thermal resistance at solid-solid junctions and localized hotspots caused by non-uniform power distribution. Both effects are amplified with shrinking device feature sizes and increasing packaging density, posing an urgent demand for high-performance thermal management materials.

2.1. Interfacial thermal resistance in electronic packaging

When two nominally flat solid surfaces are brought into mechanical contact, the actual solid-solid contact area is typically much smaller than the nominal contact area due to surface roughness and asperities [1]. The remaining interfacial gaps are filled with ambient air, which exhibits a low thermal conductivity of approximately 0.026 W/m·K at 25 °C. These trapped air gaps introduce additional thermal resistance, resulting in temperature drops across the interface and limiting heat transfer from the heat-generating die to the heat sink.

In this regard, interfacial thermal resistance can represent a significant fraction of the total thermal resistance in electronic cooling assemblies. The main role of thermal interface materials is to replace air-filled gaps and accommodate surface irregularities, thereby creating a continuous heat conduction pathway between contacting surfaces.

2.2. Localized heat generation and thermal spreading

In addition to interfacial thermal resistance, localized heat generation represents another critical challenge in advanced electronic packaging. Modern processors exhibit highly non-uniform power distributions across the die surface, where computational cores, memory controllers, and accelerator units generate heat at substantially different rates. These variations create microscale hotspots with heat fluxes far exceeding the chip-level average. For advanced AI accelerators, reported extreme hotspot heat flux values can exceed 2000 W/cm^2 in localized microscale regions under transient peak loads [1]. Such intense local heating induces large temperature gradients and thermomechanical stresses, potentially accelerating material degradation and reducing device reliability. Moreover, localized hotspots remain difficult to mitigate using conventional bulk cooling approaches because thermal spreading resistance in heat spreaders and substrates limits efficient heat redistribution and targeted heat removal [3].

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2.3. Requirements for high-performance thermal materials

To address these thermal challenges, thermal management materials for high-density computing must meet a combination of performance and engineering requirements. High thermal conductivity is the fundamental requirement, with practical TIMs generally targeting through-plane thermal conductivity above ~5–20 W/m·K to minimize interfacial temperature rise, while high in-plane conductivity is required for efficient lateral heat spreading from localized hotspots. Beyond thermal conductivity, ultra-thin form factors, typically within the tens to hundreds of micrometers range, are essential for integration into advanced packaging architectures and high-density server designs. Meanwhile, electrical insulation capability is critical, particularly for dielectric TIMs, to prevent short-circuit risks and ensure packaging reliability. In addition, long-term operational stability requires maintaining thermal performance during multi-year service periods under elevated operating temperatures (typically ~60–85 °C at the device or package level) and repeated thermal cycling, without significant degradation or performance drift. In practice, manufacturability, scalability, and cost compatibility with high-volume production remain key considerations for the practical deployment of advanced thermal materials in data center systems.

3. Thermal interface materials: from conventional composites to nanostructured systems

TIMs can be broadly divided into conventional composite systems and advanced nanostructured materials according to their structural features and heat transfer strategies. This section examines their compositions, interfacial transport mechanisms, and key factors limiting thermal performance.

3.1. Traditional composite-based thermal interface materials

Traditionally, conventional TIMs have been widely employed in electronic cooling applications for decades, with common forms including thermal pastes, greases, gap pads, and phase-change materials. In particular, these materials are composed of a polymer or oil matrix containing thermally conductive fillers. Unlike interfacial TIMs, however, phase-change materials are mainly applied in system-level thermal management for passive heat storage and peak load mitigation rather than direct heat transfer across interfaces [4].

Among these systems, commonly used fillers include inorganic ceramics such as aluminum oxide and hexagonal boron nitride, as well as metals such as silver and copper. By incorporating such fillers, the effective thermal conductivity of the low-conductivity matrix can be improved. Nevertheless, conventional randomly dispersed particle-filled TIMs typically achieve thermal conductivities in the range of approximately 10-12 W/m·K [1]. This limitation is primarily attributed to the non-uniform filler distribution and abundant filler-matrix interfaces, which introduce phonon scattering and hinder the formation of efficient heat conduction networks.

3.2. Alignment strategies for nanostructured TIMs

With the integration of one-dimensional and two-dimensional nanomaterials, TIM performance has been significantly enhanced through improved thermal transport pathways. Among these approaches, controlled filler orientation has emerged as an effective strategy, in which nanoscale conductive fillers are aligned along the heat transport direction through methods such as electric-field-assisted assembly, magnetic alignment, or mechanical stretching during fabrication.

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As shown in Figure 1, these oriented architectures create continuous thermal transport networks within the matrix, reducing phonon scattering and improving through-plane thermal conductivity compared with randomly dispersed composites [1]. For example, vertically aligned carbon nanotube arrays and aligned graphene-based structures have exhibited improved heat transport by providing directional conduction pathways [5]. And these structural designs represent promising approaches for overcoming the thermal transport limitations of conventional composite TIMs.

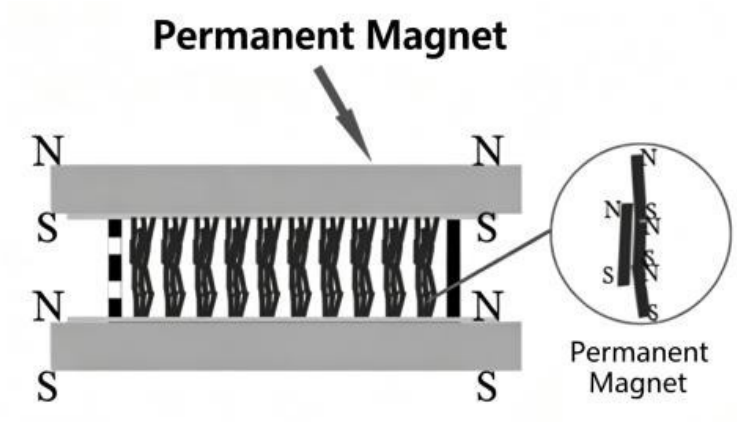


Figure 1. Oriented low-dimensional filler architectures for enhanced thermal transport

3.3. Two-dimensional nanomaterial thermal interface materials

As emerging candidates for advanced TIMs, two-dimensional nanomaterials represented by graphene and h-BN have attracted considerable attention due to their exceptional thermal transport capabilities and unique layered structures. Compared with conventional fillers, these materials provide ultrathin structures and directional heat transport pathways for interface thermal management.

Among these materials, graphene has been extensively investigated due to its outstanding intrinsic thermal conductivity. Consisting of a single layer of sp^2-bonded carbon atoms arranged in a hexagonal lattice, high-quality suspended monolayer graphene can exhibit an in-plane thermal conductivity of approximately 3000-5000 W/m·K at room temperature [6]. However, in practical TIM applications, graphene performance is strongly influenced by defects, grain boundaries, interlayer interactions, and fabrication processes. Accordingly, CVD graphene films, graphene papers, and graphene composites typically demonstrate lower thermal conductivity than pristine monolayer graphene while retaining advantages in heat spreading and flexibility. For multilayer graphene and graphite-derived structures, thermal anisotropy becomes more pronounced due to interlayer coupling, making them suitable for applications requiring directional heat dissipation.

In contrast, h-BN provides a complementary approach by combining high thermal conductivity with electrical insulation. Often referred to as "white graphene," h-BN possesses a similar hexagonal layered structure to graphene but consists of alternating boron and nitrogen atoms. Due to this unique structure, high-quality crystalline h-BN exhibits thermal conductivity of around 300-400 W/m·K while maintaining negligible electrical conductivity due to its wide bandgap [1, 7]. Therefore, h-BN is particularly attractive for TIM applications requiring both efficient heat transfer and electrical isolation, especially in high-density data center packaging where electrical reliability is critical.

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4. Practical challenges and application readiness of advanced thermal materials

4.1. Performance gap between intrinsic properties and practical TIMs

Despite their outstanding intrinsic thermal conductivity, 2D materials often exhibit limited thermal performance in practical TIM applications due to interfacial effects, material quality, and composite architectures.

In particular, interfacial thermal resistance between 2D materials and device components remains a major barrier to efficient heat transfer. Ideal phonon coupling between atomically thin materials and adjacent die or heat sink surfaces remains difficult to achieve, and interfacial phonon scattering can significantly reduce the effective thermal transport capability of assembled TIMs.

Meanwhile, the quality of large-scale synthesized 2D materials limits their practical performance. Compared with defect-free single-layer crystals, commercially produced materials typically contain defects, grain boundaries, and structural imperfections that introduce additional phonon scattering and reduce thermal conductivity. Moreover, composite-based TIM architectures introduce additional thermal resistance through filler-related interfaces. In filler-reinforced systems, thermal transport is affected by contact resistance between neighboring fillers and at filler-matrix interfaces, which can substantially reduce the overall thermal conductivity compared with the intrinsic properties of individual nanomaterials.

4.2. Manufacturing scalability and reliability considerations

At the production level, the large-scale fabrication of high-quality 2D materials remains challenging due to the need for specialized synthesis and processing routes, including chemical vapor deposition, high-temperature growth, and other controlled fabrication methods. Although alternative approaches like liquid-phase exfoliation can reduce production costs, achieving uniform quality, low defect density, and consistent thermal performance at industrial scales remains difficult. Consequently, the relatively high material and processing costs currently limit the adoption of advanced 2D-based TIMs in cost-sensitive high-volume server applications, with deployment mainly concentrated in high-performance and specialized systems [8].

Regarding long-term reliability, data center hardware is expected to operate continuously for 5-10 years under elevated temperatures and repeated thermal cycling. Over such prolonged service periods, nanostructured TIMs may experience issues such as filler agglomeration, interfacial delamination, matrix degradation, and thermal performance degradation. For example, conventional polymer-based TIMs can suffer from pump-out effects under thermal cycling, while composite systems may exhibit filler redistribution or weakened interfacial bonding over time. Therefore, comprehensive reliability testing under realistic operating conditions is required before the large-scale deployment of advanced nanostructured TIMs.

5. Emerging thermal management strategies beyond materials

As the thermal conductivity enhancement of conventional TIM materials approaches practical limits, further improvements in high-density data center cooling may require active regulation of heat transport mechanisms beyond material optimization. In this context, phonon engineering provides a framework for manipulating nanoscale heat transport and investigating thermal management concepts beyond conventional TIM technologies.

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At the fundamental research level, phononic crystals and thermal metamaterials aim to manipulate phonon transport in a manner analogous to the control of light in photonic systems. These concepts have enabled the exploration of advanced functions such as thermal diodes, thermal transistors, and directional heat guiding. Nevertheless, most current demonstrations are still confined to microscale experimental platforms, facing challenges such as scale mismatch with electronic packages, complex fabrication processes, limited operating bandwidth, and insufficient performance validation under practical device conditions.

Therefore, phonon-based thermal regulation remains a long-term research direction rather than an immediate replacement for advanced TIMs. Nevertheless, the combination of material engineering and active thermal transport control may provide new opportunities for overcoming the thermal constraints of post-Moore's Law computing systems. Beyond phonon-scale material engineering, data-driven cooling control provides an effective approach to mitigating thermal stress in high-density racks. Intelligent algorithms, such as deep reinforcement learning, can adapt cooling operations to real-time chip thermal loads, reducing energy consumption and limiting hotspot temperatures [9]. Such system-level control schemes can work synergistically with advanced TIM materials to achieve comprehensive thermal management for data-center hardware.

6. Conclusion

This review examines the development of thermal interface materials for high-density data centers, focusing on the transition from conventional composite TIMs to nanostructured systems and two-dimensional nanomaterial-based solutions. The thermal bottlenecks in advanced electronic packaging, including interfacial thermal resistance, localized hotspots, and limited heat transport pathways, are analyzed to clarify the requirements for next-generation thermal management materials. The results indicate that graphene, h-BN, and other low-dimensional nanomaterials provide advantages in thermal transport, structural flexibility, and interface engineering, offering promising solutions for high-density computing applications. However, their practical deployment remains constrained by the gap between intrinsic material properties and device-level performance, together with challenges in scalable fabrication, interface optimization, and long-term reliability validation. This review is also limited by the lack of standardized evaluation methods and insufficient long-term reliability data under realistic data center operating conditions, which complicate comparisons between laboratory-scale materials and practical applications. Future research should focus on scalable manufacturing, advanced interface engineering, and reliable performance assessment, while integrating emerging approaches such as phonon engineering to develop next-generation thermal management strategies for high-density and energy-efficient data centers.

References

[1] Tu, Y., Liu, B., Yao, G., Luo, H., Jia, X., Du, J., & Xu, C. (2024). A review of advanced thermal interface materials with oriented structures for electronic devices. *Electronics, 13*(21), 4287. https://doi.org/10.3390/electronics13214287.

[2] Khalaj, A. H., & Halgamuge, S. K. (2017). A review on efficient thermal management of air-and liquid-cooled data centers: From chip to the cooling system. *Applied Energy, 205*, 1165–1188. https://doi.org/10.1016/j.apenergy.2017.08.037.

[3] Garimella, S. V., Fleischer, A. S., Murthy, J. Y., Keshavarzi, A., Prasher, R., Patel, C., ... & Raad, P. E. (2008). Thermal challenges in next-generation electronic systems. *IEEE Transactions on Components and Packaging Technologies, 31*(4), 801–815. https://doi.org/10.1109/TCAPT.2008.2001197.

DOI: 10.54254/2755-2721/2026.37529

[4] Skach, M., Aurora, M., Hsu, C. H., Li, Q., Tullsen, D., Tang, L., & Mars, J. (2017). Thermal time shifting: Decreasing datacenter cooling costs with phase change materials. *IEEE Internet Computing*. https://doi.org/10.1109/MIC.2017.2911418.

[5] Tong, T., Zhao, Y., Delzeit, L., Kashani, A., Meyyappan, M., & Majumdar, A. (2007). Dense vertically aligned multiwalled carbon nanotube arrays as thermal interface materials. *IEEE Transactions on Components and Packaging Technologies, 30*(1), 92–100. https://doi.org/10.1109/TCAPT.2007.892079.

[6] Balandin, A. A., Ghosh, S., Bao, W., Calizo, I., Teweldebrhan, D., Miao, F., & Lau, C. N. (2008). Superior thermal conductivity of single-layer graphene. *Nano Letters, 8*(3), 902–907. https://doi.org/10.1021/nl0731872

[7] Chen, H., Ginzburg, V. V., Yang, J., Yang, Y., Liu, W., Huang, Y., ... & Chen, B. (2016). Thermal conductivity of polymer-based composites: Fundamentals and applications. *Progress in Polymer Science, 59*, 41–85. https://doi.org/10.1016/j.progpolymsci.2016.03.001

[8] Prasher, R. (2006). Thermal interface materials: Historical perspective, status, and future directions. *Proceedings of the IEEE, 94*(8), 1571–1586. https://doi.org/10.1109/JPROC.2006.879796

[9] Li, Y., Wen, Y., Tao, D., & Guan, K. (2019). Transforming cooling optimization for green data center via deep reinforcement learning. *IEEE Transactions on Cybernetics, 50*(5), 2002–2013. https://doi.org/10.1109/TCYB.2019.2927410