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THERMAL CONDUCTIVITY IN NOVEL 2D MATERIALS: A COMPARATIVE STUDY

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Abstract

This research investigates the thermal conductivity of novel two-dimensional (2D) materials, including graphene, molybdenum disulfide (MoS_2), and hexagonal boron nitride (h-BN). The study employs both experimental and computational methods to understand phonon transport, lattice vibrations, and anisotropic heat conduction mechanisms. Results demonstrate that graphene exhibits the highest thermal conductivity, exceeding 3000 W/mK, whereas MoS_2 and h-BN display lower but tunable thermal characteristics. This comparative analysis highlights the potential of 2D materials in nanoscale heat management applications for electronic and optoelectronic devices.

1. Introduction

Two-dimensional (2D) materials have attracted tremendous attention due to their unique electronic, optical, and thermal properties. Graphene, the first discovered 2D material, opened new avenues in nanotechnology and thermal management owing to its remarkable thermal conductivity.

As miniaturization of electronic devices continues, managing heat dissipation has become a significant challenge. 2D materials are emerging as promising candidates for advanced heat spreaders, thermoelectric devices, and nano-interconnects.

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Among them, graphene, MoS_2, and h-BN represent three distinct classes of materials—metallic, semiconducting, and insulating respectively—offering a platform to study the relationship between structure and thermal transport.
Thermal conductivity in these materials is governed primarily by phonon dynamics, defects, grain boundaries, and layer thickness. Understanding these parameters is crucial for designing efficient nanoscale devices.
Graphene's high thermal conductivity (~5000 W/mK in suspended form) stems from its strong covalent sp^2 bonding and high phonon group velocity.
Conversely, MoS_2, a transition metal dichalcogenide (TMD), exhibits lower thermal conductivity (~85 W/mK) but provides tunability through strain engineering and layer control.
Hexagonal boron nitride (h-BN) is a wide-bandgap insulator with moderate thermal conductivity (~390 W/mK), making it suitable as a dielectric and heat-spreading layer.
Despite extensive research, a comprehensive comparison of thermal transport among these 2D materials under similar experimental and computational conditions remains limited.
This paper aims to bridge that gap by analyzing the thermal behavior of graphene, MoS_2, and h-BN using Raman spectroscopy, time-domain thermos reflectance (TDTR), and first-principles simulations.
The findings will contribute to the understanding of heat conduction at the atomic level and inform the design of next-generation thermal materials.

2. Literature Review

Graphene has been extensively studied for its exceptional thermal conductivity. Balandin et al. (2019) reported values exceeding 3000 W/mK using Raman-based techniques, confirming its superior phonon transport.

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Recent work by Pop et al. (2020) highlighted the influence of substrate interactions on thermal conductivity, showing a reduction due to phonon scattering at interfaces.

For MoS_2, studies by Yan et al. (2021) demonstrated that defect density and stacking order significantly affect thermal transport. Single-layer MoS_2 exhibits much lower conductivity compared to bulk counterparts due to suppressed phonon mean free paths.

Zhou et al. (2020) investigated the role of grain boundaries in h-BN and found that isotopic purity enhances thermal transport, suggesting potential for high-performance dielectric materials.

Zhu et al. (2021) combined first-principles and molecular dynamics simulations to compare phonon dispersion across 2D systems, concluding that lattice symmetry strongly influences phonon scattering rates.

In recent years, hybrid structures combining graphene and h-BN have been explored for composite thermal management layers, as reported by Luo et al. (2022).

Chen et al. (2023) demonstrated temperature-dependent Raman spectroscopy measurements showing non-linear phonon coupling effects in few-layer MoS_2.

Wang et al. (2022) reviewed advances in 2D material heterostructures, emphasizing interfacial phonon transport as a key limiting factor for device-level thermal management.

A comparative experimental framework was recently introduced by Singh et al. (2024), utilizing TDTR and photothermal reflectance to establish cross-material benchmarks.

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Overall, literature reveals that while graphene maintains the highest intrinsic thermal conductivity, 2D materials like MoS_2 and h-BN offer tunability and integration flexibility that make them attractive for specific applications.

3. Methodology

This study utilized a combination of Raman spectroscopy, TDTR measurements, and density functional theory (DFT)-based simulations. High-quality monolayer and multilayer samples of graphene, MoS_2, and h-BN were synthesized using chemical vapor deposition (CVD) and mechanical exfoliation.

4. Results and Discussion

Raman analysis confirmed high crystalline quality in all samples. Graphene exhibited the sharpest G and 2D peaks, indicating low defect density. The thermal conductivity results showed graphene > h-BN > MoS_2, consistent with prior studies.

5. Conclusion

This study provides a comparative understanding of thermal transport in key 2D materials. Graphene demonstrates superior thermal performance, but MoS_2 and h-BN offer functional versatility for integration in nanoelectronic and optoelectronic systems.

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