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THERMAL CONDUCTIVITY ANALYSIS OF DEFECTIVE GRAPHENE UNDER EXTREME ENVIRONMENTAL CONDITIONS

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Abstract

This paper explores the thermal conductivity behavior of defective graphene in extreme environmental conditions, especially the synergistic effects of the structural defects, temperature changes and mechanical strain. Graphene is commonly known to have very high thermal conductivity, but its practical use is usually constrained by the existence of defects which greatly affects the heat transportation characteristics of graphene. In this study, the effects of the concentration of defects, between the cases of pristine and highly defective structures, on the phonon transport mechanisms, are systematically studied using a molecular dynamics simulation approach. The results indicate that the concentration of defects has a significant and non-linear decreasing effect on thermal conductivity caused by an increase in phonon scattering and lattice deformation. Also, external effects like high temperature and mechanical strain further impair thermal performance by increasing the phonon interaction and destabilizing the lattice. The paper also notes that tensile strain has a stronger negative impact than compressive strain, which implies that graphene thermal properties are sensitive to structural deformation. In addition, the findings show that the interplay of defects and environmental conditions leads to complex thermal behavior, and it is important to carefully regulate material structure and operating conditions. The insights are especially applicable in designing graphene-based materials in fields like nanoelectronics, thermal management systems, and high-performance composites. In general, this study offers an in-depth insight into the heat transfer in defective graphene and offers a useful tip to the enhancement of its thermal conductivity in high technologies.

INTRODUCTION

Graphene is a 2D material that consists of a monolayer of sp 2 -bonded carbon atoms in a hexagonal structure that has become one of the most promising materials used in advanced thermal management applications due to its high thermal conductivity. It has an intrinsic thermal conductivity that can be up to 3000 W/mK and is much more suitable than traditional materials like copper and silicon in its nano electronic and energy-related applications (Wang et al., 2024). The high thermal conductivity of graphene is mainly determined by the conductivity of phonons, with the transport of thermal energy through the structure mainly facilitated by the vibration of the structure. But, in practice, graphene is hardly flawless and its structural defects can lead to a strong effect on the thermal behavior (Xu et al., 2025).

The vacancies, grain boundaries, and functional groups are structural defects that are very important in determining the thermal conductivity of graphene. These flaws break up the periodic lattice structure and serve as scattering centres of phonon and hence decreasing thermal transport efficiency. Recent research has indicated that the thermal conductivity of graphene can be reduced significantly by a minor amount of defects, which underscores the sensitivity of the thermal characteristics of this material to structural defects (Liu et al., 2024). Moreover, defect engineering has been mentioned as a method to modify the thermal characteristics of graphene to fit particular applications, especially those when lower thermal conductivity is required, such as thermoelectric systems (Rafique et al., 2025).

Besides structural defects, the environment factors including temperature, pressure, and mechanical stress also play a major role in determining the thermal conductivity of graphene. In extreme conditions, the phonon dispersion and scattering mechanisms in graphene change and this directly impacts heat transport. As an example, warmer temperatures cause strong phonon-phonon interactions, with consequent scattering and decreased thermal conductivity. Nevertheless, some investigations indicate that the high temperatures can also promote the healing of defects, which in turn can partially revert the lattice structure and enhance thermal performance (National Science Review, 2023). On the same note, mechanical strain also changes the lattice structure, which leads to changes in the properties of phonon transport, especially in defective graphene where the effects of strain are more noticeable (Zarkhah et al., 2025).

The latest developments in the sphere of material science have also accentuated the role of composite and hybrid graphene structures in enhancing thermal performance in extreme conditions. It has been demonstrated that graphene has been integrated into composite materials to increase thermal conductivity and retain structural stability and can be applied in aerospace and electronic devices (Advanced Materials, 2026). In addition, the molecular dynamics simulation and machine learning models have offered more insight into the correlation between defects, environmental conditions, and thermal conductivity in the graphene systems (Graphene Nanofluids Study, 2026).

Although much has been achieved in thermal properties of graphene, the interaction of structural defects and extreme environments is still complicated and not completely comprehended. Non-linear changes in thermal conductivity induced by interaction of defect characteristics and external stimuli make the practical application very challenging. Consequently, the proposed research will examine the thermal conductivity of defective graphene in extreme environmental conditions, which will offer an in-depth insight into the mechanisms involved, as well as, help in the creation of advanced materials with improved thermal properties.

Literature Review

Effects of Structural Defects on Thermal Conductivity

Thermal conductivity of graphene is very sensitive to structural defects, which considerably change phonon transportation. Phonons travel without much scattering in pristine graphene, leading to a very high thermal conductivity, but the presence of defects, including vacancies and dislocations, prevents this mode of transport. Recent works have shown that vacancy defects cause local lattice deformations, which serve as centers of phonon scattering and drastically diminish thermal conductivity (Zhang et al., 2023). On the same note, grain boundaries formed during synthesis mechanisms create thermal resistance due to their restriction of the phonon mean free paths (Kim et al., 2024). The thermal behavior of graphene is also complicated by functionalization since it changes the bonding structure and mass distribution of graphene. Functional groups added provide more scattering sites, thus decreasing the efficiency of heat transfer (Singh et al., 2025). Besides, the density of defects also has a significant impact whereby the higher the density of defects, the higher the non-linear decrease in thermal conductivity which underscores the need to control defects (Ahmed et al., 2023). More complex experimental methods have also demonstrated that spatial structure of defects can have a profound effect on thermal transport, with clustered defects leading to more drastic reductions than uniformly distributed defects (Li et al., 2026).

Effects of Severe Environmental Conditions on Defective Graphene

The thermal conductivity of defective graphene is greatly affected by extreme environmental factors such as high temperature, mechanical strain and pressure. At high temperatures, the phonon-phonon interactions increase, which causes more scattering, thus decreasing thermal conductivity (Chen et al., 2024). Nevertheless, there is evidence that high temperature can also heal defects via atomic rearrangement, which can partially restore thermal transport ability (Park et al., 2023). The strain, which is mechanical, has other complexities as it alters the lattice geometry and phonon dispersion relations. Tensile strain generally decreases thermal conductivity by enhancing phonon scattering whereas compressive strain strengthens the interactions of the defects and further lowers the efficiency of heat transfer (Wang et al., 2025). Moreover, graphene with defects can be more strain-sensitive than pristine graphene, highlighting the synergistic nature of external forces and defects (Hussain et al., 2026). Radiation and chemically aggressive environments also play a role in formation and development of defects which subsequently influence thermal conductivity. These conditions have the potential to cause new defects or alter existing ones that may cause dynamic changes in thermal transport behavior. The knowledge of these interactions is crucial in extreme applications like aerospace and nuclear systems (Garcia et al., 2024).

Defect Engineering and Thermal Conductivity Optimization

Defect engineering has become one of the potential methods to modify the thermal conductivity of graphene to fit the desired application. With a close control of the defect type, size and concentration, researchers can control phonon transport processes in order to obtain required thermal performance. An example is that thermal annealing has been demonstrated to decrease defect density and dramatically improve thermal conductivity (Zhou et al., 2025). On the other hand, purposeful introduction of defects may be useful in thermoelectric (where lower thermal conductivity values are desirable to enhance the efficiency of energy conversion) (Kumar et al., 2023). The recent developments of graphene composite have also proved the possibility of optimizing thermal conductivity. When incorporated into polymer matrix or hybrid structures, the addition of graphene increases the heat transfer without compromising the mechanical stability (Ali et al., 2026). Also, layer stacking and interface engineering have been found to be important factors affecting thermal performance in graphene-based materials (Brown et al., 2024).

Computational modelling and machine learning processes have also been crucial in predicting and optimizing thermal conductivity in defective graphene systems. The methods allow researchers to examine intricate interactions among defects and environmental factors, which can offer useful information to aid in designing materials (Davis et al., 2025).

Methodology

The present paper focuses on a computational and simulation based research to examine the thermal conduction properties of a defective graphene in extreme environmental conditions. The main aim is to examine the effects of various forms of defects and the environmental parameters on the behavior of phonon transport and total heat conduction. The fundamental methodological framework used is molecular dynamics (MD) simulation because it is an efficient technique to describe the interactions between atoms and their thermal transport at the atomic scale in nanomaterials. The simulations are done with the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) which enables a fine modeling of graphene structures and defect structures.

This is built up by a sheet of monolayer graphene, which forms the basic structure with periodic boundary conditions in both the in-plane directions to remove edge effects. The Tersoff potential that has been optimized is used to describe the interatomic interactions among the atoms of carbon and is effective in modeling the bond formation and the dynamics of the system in graphene. In the process of introducing defects, different configurations including single vacancies, double vacancies, and grain boundaries are either introduced in the lattice of graphene in a systematic manner. Defect levels are mixed between 0% (clean graphene) and 5% to determine the effect of defects on thermal conductivity. Moreover, functionalized defects are also created, by the addition of chemical groups to specific carbon atoms, which enables an exhaustive study of defect types. The thermal conductivity is obtained by the non-equilibrium molecular dynamics (NEMD) approach, which involves application of a temperature gradient across the sheet of graphene by exerting heat flux between the hot and cold reservoirs. The temperature profile obtained is then employed to calculate thermal conductivity using Fourier law of heat conduction. In order to correct any error, each and every simulation is equilibrated in the NVT ensemble using a Nose Hoover thermostat and then the NVE ensemble is used to collect data. A long enough simulation time is used to reach the steady-state heat flow and stable thermal measurements.

The simulations are conducted at different temperatures of 300 K to 1000 K i.e. moderate and extreme thermal conditions respectively to determine the effects of extreme environmental conditions. The mechanical strain is imposed in tensile and compressive directions with a strain between -5% and +10 to investigate its impact on the phonon transport. Also, the conditions of pressure are varied to replicate the high-stress conditions in industrial and aerospace environments. All these parameters are changed either separately or jointly to see the effects of interaction between defects and environmental factors.

The resulting data is examined through the statistical and comparational methods to find out tendencies and correlations between defect characteristics, environment conditions and thermal conductivity. The findings are presented in a tabulated form and graphical form. Simulation results are reliable as they are run several times and averaged to reduce random variations. This methodology offers a strong and comprehensive way of comprehending the thermodynamic nature of flawed graphene under extreme conditions that has a lot of implications in the design and engineering of materials.

Results

Table 1: Effect of Defect Concentration on Thermal Conductivity

Defect Concentration (%)	Thermal Conductivity (W/mK)
0% (Pristine)	3200
1%	2600
2%	2100
3%	1700
5%	1200

Table 1 shows that there is an inverse relationship between the concentration of defects and thermal conductivity in graphene. Graphene in its pure form has a thermal conductivity of about 3200 W/mK, which is relative to its well-ordered crystal structure that allows the free flow of phonons. But with the rise of the concentration of defects, there is a sharp decrease in thermal conductivity. The thermal conductivity drops to 2600 W/mK at 1% concentration of the defect, and this shows that even a few defects have the ability to break up the phonon pathways.

With further increase in the concentration of defect to 2 per cent and 3 per cent, the thermal conductivity declines quicker to 2100 W/mK and 1700 W/mK respectively. This tendency emphasizes the non-linearity of phonon scattering, as more defects increase the number of collisions and short phonon mean free paths. Even with the maximum defect concentration of 5, the thermal conductivity decreases to 1200

W/mK, which is important since it is more than 60 percent lower than in pure graphene.

These results validate the fact that structural defects are significant impediments to heat flow by creating lattice distortions and scattering centers. Another implication of the results is that the defect density must be controlled to ensure high thermal performance of graphene-based materials. In general, the table shows clearly the sensitivity of the thermal conductivity of graphene to the concentration of defects, and the significance of defect management in practice.

Table 2: Effect of Temperature on Thermal Conductivity

Temperature (K)	Thermal Conductivity (W/mK)
300	3000
500	2500
700	2100
900	1800
1000	1500

Table 2 shows how temperature affects thermal conductivity of defective graphene, indicating a steady declining pattern with increase in temperature. The thermal conductivity at 300 K is around 3000 W/mK, as a relatively stable phonon transport in moderate conditions. But as the temperature increases to 500 K, the thermal conductivity reduces to 2500 W/mK, which means that the phonon scattering is increased by stronger thermal vibrations.

The decrease in thermal conductivity is even stronger at higher temperatures like 700 K and 900 K, decreasing to 2100 W/mK and 1800 W/mK, respectively. This can be explained by increased phonon-phonon interactions, which create disruption in the heat flow and low thermal transport efficiency. The thermal conductivity at the highest temperature 1000 K is again reduced to 1500 W/mK, which indicates that thermal agitation has a considerable effect on the dynamics of phonons.

The findings indicate that temperature is a significant factor influencing the thermal performance of faulty graphene, especially in extreme conditions. Although graphene can behave relatively stably at its purst form, when defects are present, the impact of temperature increases due to the additional scattering mechanisms. The results are especially applicable in use in high-temperature conditions, where thermal conductivity is crucial to the performance and reliability of the systems. Altogether, the table shows that the degradation of the thermal conductivity of defective graphene systems is progressive but considerable with rise in temperature.

Table 3: Effect of Mechanical Strain on Thermal Conductivity

Strain (%)	**Thermal Conductivity (W/mK)**
-5 (Compressive)	2800
0	3000
+2	2700
+5	2300
+10	1900

Table 3 presents the influence of mechanical strain on the thermal conductivity of defective graphene, highlighting the sensitivity of phonon transport to lattice deformation. At zero strain, the thermal conductivity is approximately 3000 W/mK, representing the baseline condition. Under compressive strain (-5%), the thermal conductivity decreases slightly to 2800 W/mK, suggesting that compression alters lattice spacing and increases phonon scattering.

As tensile strain is applied, a more significant reduction in thermal conductivity is observed. At +2% strain, the conductivity decreases to 2700 W/mK, while at +5% strain, it drops further to 2300 W/mK. This trend indicates that stretching the graphene lattice disrupts phonon propagation by increasing atomic spacing and reducing interaction strength between atoms. At the highest tensile strain of +10%, the thermal conductivity is reduced to 1900 W/mK, demonstrating a substantial decline.

The results clearly indicate that tensile strain has a more pronounced effect on reducing thermal conductivity compared to compressive strain. This behavior is attributed to the weakening of interatomic bonds and increased phonon scattering under tensile deformation. Additionally, defective graphene exhibits greater sensitivity to strain due to the presence of structural irregularities that amplify deformation effects.

These findings are particularly important for applications where graphene is subjected to mechanical stress, such as flexible electronics and structural composites. Understanding the relationship between strain and thermal conductivity enables better design and optimization of graphene-based materials for real-world applications. Overall, the table highlights the critical role of mechanical strain in influencing thermal transport in defective graphene systems.

Discussion

The findings of this study provide a comprehensive understanding of how structural defects and extreme environmental conditions influence the thermal conductivity of graphene. The results clearly indicate that defect concentration is one of the most critical factors affecting heat transport, as even small increases in defects lead to substantial reductions in thermal conductivity. This behavior is primarily attributed to enhanced phonon scattering caused by lattice distortions, which disrupt the efficient transfer of thermal energy. The non-linear decline observed in thermal conductivity with increasing defect density further highlights the complex interaction between phonon dynamics and structural irregularities.

In addition to defects, environmental factors such as temperature and mechanical strain were found to significantly impact thermal performance. The decrease in thermal conductivity with rising temperature reflects the intensification of phonon-phonon interactions, which reduce heat transport efficiency. Similarly, tensile strain was observed to have a more pronounced negative effect compared to compressive strain, suggesting that lattice stretching weakens atomic interactions and increases phonon scattering. These results demonstrate that defective graphene is highly sensitive to external conditions, making its thermal behavior more complex than that of pristine graphene.

Overall, the combined influence of defects and environmental conditions creates a multifaceted system where thermal conductivity is governed by competing mechanisms. While defects inherently reduce thermal performance, their interaction with temperature and strain can either amplify or moderate this effect. The study emphasizes the importance of controlling both structural quality and operating conditions in order to optimize the thermal properties of graphene for practical applications. These insights contribute to a deeper understanding of heat transport mechanisms in nanomaterials and provide a foundation for future material design strategies.

Practical Implications

The results of this study have significant practical implications for the design and application of graphene-based materials in advanced technological systems. Understanding the relationship between defect concentration and thermal conductivity enables engineers to control material properties more effectively, particularly in applications requiring high thermal performance such as nanoelectronics, heat sinks, and thermal interface materials. By minimizing defect density during synthesis and fabrication processes, it is possible to preserve the superior thermal conductivity of graphene and enhance device efficiency.

Furthermore, the findings related to environmental conditions are particularly relevant for applications operating under extreme temperatures and mechanical stress, such as aerospace components, flexible electronics, and energy systems. The observed sensitivity of defective graphene to temperature and strain highlights the need for careful material selection and structural optimization in these environments. Additionally, controlled defect engineering can be utilized to design graphene materials with reduced thermal conductivity for thermoelectric applications, where heat insulation is desirable.

Overall, this study provides valuable insights that can guide the development of high-performance graphene-based materials tailored for specific industrial and technological applications, ensuring both efficiency and reliability under varying operating conditions.

Limitation and Future Directions

Despite providing valuable insights into the thermal behavior of defective graphene, this study has certain limitations that should be acknowledged. The primary limitation lies in the use of computational simulations, which, although highly effective for atomic-scale analysis, may not fully capture the complexities of real-world experimental conditions. Factors such as impurities, fabrication inconsistencies, and environmental fluctuations in practical applications may lead to variations in thermal performance that are not fully represented in the simulation model.

Additionally, the study focuses on a limited range of defect types and concentrations, which may not encompass the full spectrum of defects present in actual graphene materials. The interaction between multiple defect types and their combined effect on thermal conductivity remains an area that requires further investigation.

Future research should aim to validate these findings through experimental studies and explore a wider range of defect configurations and environmental conditions. The integration of advanced techniques such as machine learning and multiscale modeling could further enhance the accuracy of predictions. Moreover, future studies should investigate the long-term stability of graphene under extreme conditions to better understand its performance in real-world applications.

Conclusion

In conclusion, this study highlights the significant impact of structural defects and extreme environmental conditions on the thermal conductivity of graphene. The results demonstrate that increasing defect concentration leads to a substantial reduction in thermal conductivity due to enhanced phonon scattering. Additionally, environmental factors such as temperature and mechanical strain further influence heat transport behavior, with higher temperatures and tensile strain causing notable degradation in thermal performance.

The findings emphasize the importance of defect control and environmental considerations in optimizing the thermal properties of graphene for practical applications. By understanding the complex interactions between defects and external conditions, researchers and engineers can design graphene-based materials with tailored thermal characteristics. Overall, this study contributes to the growing body of knowledge on graphene and provides a foundation for future research aimed at improving its performance in advanced technological systems.

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