

Research Article

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Differential study on the thermal-physical properties of metal and its oxide nanoparticle-formed nanofluids: Molecular dynamics simulation investigation of argon-based nanofluids

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Abstract: The influence of nanoparticle shape, volume fraction, and temperature on the thermal properties of nanofluids plays a pivotal role in engineering applications. However, there remains a considerable lack of systematic research comprehensively considering these factors to study the similarities and differences in the thermal properties of nanofluids composed of metals and their oxides and to conduct in-depth analyses of their internal mechanisms and characteristics. In this study, molecular dynamics simulations were conducted, employing reversing perturbation non-equilibrium molecular dynamics and non-equilibrium molecular dynamics methods. The thermal conductivity and viscosity of Al-Ar and Al_2O_3 -Ar nanofluids were thoroughly investigated under the various influencing factors. Results reveal that under identical conditions, the thermal conductivity of Al-Ar nanofluid surpasses that of Al_2O_3 -Ar nanofluid, exemplified by values such as 0.1832 W/m K (Al-Ar, 1.5%, cylinder, 86 K) versus 0.17745 W/m K (Al_2O_3 -Ar, 1.5%, cylinder, 86 K). Furthermore, the viscosity of Al-Ar nanofluid is lower than that of Al_2O_3 -Ar nanofluid, demonstrated by values such as 0.0004882 Pa S (Al-Ar nanofluid, 86 K, 2.5%, platelets) compared to 0.000975 Pa S (Al_2O_3 -Ar nanofluid, 86 K, 2.5%, platelets). Subsequently, this study analyzed the difference in thermal conductivity between the

two nanofluids from the perspective of microscale interface heat conduction by comparing the phonon density of states curves of Al, Ar, and Al_2O_3 in the two nanofluids for overlap. Subsequently, through radial distribution function analysis, the viscosity difference between Al-Ar and Al_2O_3 -Ar nanofluids is explained based on nanofluid-solid interface and microstructural considerations. This research addresses the comprehensive lack of comparative studies on the thermal properties of nanofluids formed by metals and their oxides. The internal mechanisms underlying the thermal property differences of nanofluids formed by metals and their oxides were revealed from a microscopic perspective, which holds significant implications for the engineering applications of nanofluids.

Keywords: nanofluid, metals and their oxides, molecular dynamics simulation, phonon density of states, radial distribution function

1 Introduction

Nanofluids are functional fluids formulated by dispersing metal, metal oxide, or other non-metal nanoparticles (NPs) with exceptional suspension capabilities into a base fluid (BF), thereby achieving superior thermophysical properties. Due to their outstanding thermal characteristics, nanofluids have recently received widespread attention in fields requiring high heat transfer efficiency, such as microelectronics cooling, air conditioning, mechanical friction, and other related applications [1–5].

As mentioned earlier, nanofluids exhibit exceptional thermophysical properties, among which the most notable are their high thermal conductivity [6–9] and acceptable viscosity characteristics compared to heat transfer fluids formed with micrometer-sized particles in BFs. These

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Differential Thermal Investigation Of Cl

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Table of Contents Differential Thermal Investigation Of Cl

1. Understanding the eBook Differential Thermal Investigation Of Cl
 - The Rise of Digital Reading Differential Thermal Investigation Of Cl
 - Advantages of eBooks Over Traditional Books
2. Identifying Differential Thermal Investigation Of Cl
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Differential Thermal Investigation Of Cl
 - User-Friendly Interface
4. Exploring eBook Recommendations from Differential Thermal Investigation Of Cl
 - Personalized Recommendations
 - Differential Thermal Investigation Of Cl User Reviews and Ratings
 - Differential Thermal Investigation Of Cl and Bestseller Lists
5. Accessing Differential Thermal Investigation Of Cl Free and Paid eBooks
 - Differential Thermal Investigation Of Cl Public Domain eBooks
 - Differential Thermal Investigation Of Cl eBook Subscription Services
 - Differential Thermal Investigation Of Cl Budget-Friendly Options

6. Navigating Differential Thermal Investigation Of CI eBook Formats
 - ePub, PDF, MOBI, and More
 - Differential Thermal Investigation Of CI Compatibility with Devices
 - Differential Thermal Investigation Of CI Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Differential Thermal Investigation Of CI
 - Highlighting and Note-Taking Differential Thermal Investigation Of CI
 - Interactive Elements Differential Thermal Investigation Of CI
8. Staying Engaged with Differential Thermal Investigation Of CI
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Differential Thermal Investigation Of CI
9. Balancing eBooks and Physical Books Differential Thermal Investigation Of CI
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Differential Thermal Investigation Of CI
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Differential Thermal Investigation Of CI
 - Setting Reading Goals Differential Thermal Investigation Of CI
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Differential Thermal Investigation Of CI
 - Fact-Checking eBook Content of Differential Thermal Investigation Of CI
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
 - Integration of Multimedia Elements

- Interactive and Gamified eBooks

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