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Study on Ammonia Copper Nanocomposite Thermal Performance in Cavity Nanochannels under Electric Field

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Abstract:
Enhancing the performance of thermal exchange systems remains a significant challenge for technical professionals and system architects. To address this, introducing nanoscale particles into primary fluids has emerged as a promising passive approach, offering enhanced thermal conductivity properties and enabling more compact heating and cooling systems. This study utilizes molecular-scale simulation techniques to examine the thermal transport characteristics of copper nanoparticles interacting with ammonia refrigerant in a nanoconfined system. The findings reveal that as the frequency of the applied electric field rises from 0.11/ps to 0.51/ps, the time required for phase change extends from 2 to 3 nanoseconds, while heat transfer efficiency drops from 0.76 W/mK to 0.72 W/mK. Furthermore, the study explores the impact of different structural designs of cavities—closed, round, and box-shaped—on the microscopic and heat-related properties of the simulated samples. Among these, the cubic cavity demonstrates the maximum heat transfer efficiency, reaching 0.80 W/mK. The analysis also considers different atomic cavity types, including Hermitian, spherical, and cubic structures. The extent and duration of the phase change are 65%, 66% and 68%, and 2.88 nanoseconds, 2.87 nanoseconds and 2.85 nanoseconds, respectively.

Keywords: Efficiency of heat transfer system; Nanoparticles; Molecular dynamics simulation; Electric field frequency; Thermal behavior of cavity structure

INTRODUCTION

In the industrial field, the challenges associated with heating and cooling systems have long been a significant concern for numerous industries and researchers. All links of industrial production, whether it is the operation of large machinery for heat dissipation, or the temperature control in chemical production, the efficiency, cost and safety of cooling and heating process are crucial. The existing solutions for improving heat transfer operation do improve the heat transfer level to a certain extent, as described in [1]. However, this solution has a disadvantage that can not be ignored, that is, it improves the heat transfer level by increasing the volume flow of coolant. This seems to be a direct and effective method, but it has brought new cost problems. Specifically, the pumping cost has greatly increased, as pointed out in [2]. Under the dual pressure of cost and efficiency, scientists must proactively explore innovative approaches to enhance the performance of refrigeration systems. In this process of exploration, refrigeration equipment, especially refrigerators, has become the focus of researchers [3]. They tried to use different amounts of compound (R600, R134a or R290) in the refrigerator. This attempt is not blind, because through a large number of experiments and analysis, the results show that HC/HFC has the potential to replace the traditional refrigerant R12, it also made achievements in this research direction [4]. They showed the role of the combination of R152a and R125 refrigerants in cooling. Specifically, when this compound is combined with 0.85% HFC152a, it can act as HFC12 refrigerant. However, this achievement is not perfect, its application is still facing challenges, and it also needs the support of the further development of nanotechnology [5].

After all, nano materials have significantly improved the heat transfer fluid in the modern process. Advancements in nanotechnology have revealed that dispersing nanoparticles into base fluids yields remarkable effects. Owing to the superior thermal conductivity of nanoparticles, this characteristic significantly influences the thermal properties of the base fluid, leading to an enhancement in thermal conductivity—a critical parameter for heat transfer efficiency. This phenomenon is described in detail in [6,7]. S. Bi et al. [8] conducted special research on R134a refrigerant, and they applied alumina nanoparticles to R134a refrigerant. After rigorous experimental tests, the findings indicate that with a 0.2% mass fraction of alumina nanoparticles, the energy consumption of the refrigeration system decreases by 10.2% compared to its pure state. This evidence strongly supports the positive impact of alumina nanoparticles on enhancing the heat transfer coefficient. In the study of complex molecular systems, the molecular system usually contains a very large number of atoms, which makes the research process full of challenges. The molecular dynamics (MD) simulation method came into being, which provides an effective way to solve these problems. This approach was employed to investigate relatively straightforward systems. However, with technological advancements and deeper exploration, it has evolved to analyze even the most intricate physical systems. The

progression of this methodology is well-documented in references [9,10]. Numerous researchers, including Mosavi et al. [11], Toghraie et al. [12], and Shang et al. [13], have utilized and expanded the application of molecular dynamics simulations in their respective studies. A key use of molecular dynamics simulation is to forecast the atomic and thermal characteristics of nanofluids. For instance, Hekmatifar et al. [14] extensively studied the thermal properties of Cu/Ar nanofluids using MD simulations. Through a series of simulations and computations, they determined that the thermal conductivity of Cu/Ar nanofluids is 0.016 W/mK, and the inclusion of Cu nanoparticles enhances this property. This research also highlighted that external forces applied to the system significantly influence the thermal behavior of nanofluids. Lu et al. [15] similarly employed molecular dynamics to investigate [16], arranging fluid atoms by introducing nanoparticles. During their experiments, they observed intriguing phenomena [17-18], noting that the nanoparticles altered the fluid's atomic structure and introduced voids in the density distribution, suggesting bubble formation within the atomic framework [19]. Further exploration revealed that increasing the temperature and nanoparticle concentration in the base fluid [20-21] could create regions of zero atomic density in a relatively short time. Reviewing prior studies [22], across various domains of nanotechnology [23-24] and in areas like lubrication and heat transfer [25-26], a research gap was identified: the heat transfer dynamics of ammonia refrigerant infused with copper nanoparticles remain unexplored [27-28].

To address this gap, atomistic simulations based on molecular dynamics principles were conducted to characterize the thermophysical behavior of copper nanoparticle-enhanced ammonia refrigerant under applied electric field conditions.This research also examined the effects of varying electric field frequencies and different cavity configurations (sealed, spherical, and cubic) within nanochannels on the atomic and thermal dynamics of the simulated systems. By precisely evaluating critical parameters such as phase transition values, transition durations, and thermal conductivity, a thorough and detailed understanding of the thermal behavior of the studied structures was achieved.

MOLECULAR DYNAMICS SIMULATION

These employs advanced molecular dynamics simulation methods to investigate the atomic-level characteristics and thermodynamic behavior of the refrigerant ammonia inochannels. This study aims to better understand the transport mechanisms, phase transition behaviors, and energy conversion efficiency of ammonia in confined spaces, providing a theoretical foundation for development of more efficient and environmentally friendly refrigeration technologies. To achieve this goal, we first establish a framework of accurate system equations of motion, which is based defining and solving the potential energy equations that govern the interactions between particles.

$$F_i = -\nabla_i U \tag{1}$$

In the field of physics research, especially in the study of microscopic particles, there is a generally recognized rule: the force acting on particle is usually proportional to the interatomic interaction force. This rule is an important foundation for many studies in microscopic physics. Since the force acting on each atom directly its change in motion state, in alignment with Newton's second law of motion, a direct correlation exists between the force applied to an object and the resulting acceleration it experiences and acceleration is closely related to changes in velocity Therefore, by carefully analyzing the force acting on each atom, we can obtain the velocity of each atom. In the specific research method of molecular dynamics simulation, the is even more complex and detailed. Molecular dynamics simulation is a powerful tool that helps us understand the behavior of molecules, atoms, and other microscopic particles from a microscopic. In this simulation process. The velocity-Verlet algorithm, as outlined in equations (1) and (2) [10], provides a computational framework for solving Newton's equations of motion, enabling the precise determination of particle trajectories and dynamic behavior over time.

$$r(t+\Delta t) = r(t) + \Delta t v(t) + \frac{\Delta t^2 a(t)}{2} \tag{2}$$

$$v(t+\Delta t) = v(t) + \Delta t v(t) + \frac{\Delta t\ (a(t)+a(t+\Delta t))}{2} \tag{3}$$

In the field of molecular dynamics simulations, equations (1) and (2) hold significant importance. Among them, Δt represents the step, which is a crucial parameter in molecular dynamics simulations. In this study, the focus is on specific systems, namely the interaction between aluminum particles within the wall nanoparticles in the nanofluid. For these particle interactions, the potential function is used for simulation, as expressed in equation (3) [16]. The selected interatomic formalism demonstrates distinct computational merits for modeling particulate dynamics within complex material systems. Its mathematical framework aligns more closely with the multi-physics requirements of interfacial interaction analysis, thereby

enabling rigorous characterization of metallic inclusions in constrained geometries and colloidal dispersions. This methodology proves particularly advantageous for investigating aluminum-based microstructures in confined domains while maintaining fidelity in simulating nanoscale particle behavior across heterogeneous phases. The approach facilitates precise resolution of interfacial phenomena critical for understanding phase-boundary effects in both solid-state matrices and liquid-phase nanocolloidal suspensions.

$$U_i = F_a\left(\sum_{i\neq j}\rho_\beta(r_{ij})\right)+\frac{1}{2}\sum_{i\neq j}\phi_\beta(r_{ij}) \tag{4}$$

In Eq. (3), φ_β represents the interatomic antagonism and ρ_β denotes the attractive force, while r_{ij} indicates the interparticle separation. To account for the interaction between amino acid particles and nanoparticles, the UFF force field was employed, which is a truncated formulation of the Lennard-Jones formalism, as shown in Eq. (4). [12]:

$$U_{LJ} = 4\varepsilon\left[(\frac{\sigma}{r})^{12}-(\frac{\sigma}{r})^{6}\right] \tag{5}$$

In the representation of Eq. (4), ε represents the characteristic energy minimum of the interparticle potential landscape, and σ defines the radial cutoff threshold of potential energy dissipation. According to the definitions (Eqs. (5) and (6)), the established quantitative parameters of σ and ε, and the available empirical dataset in Table 1, we have successfully simulated the interaction between particles inside the box.

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} \tag{6}$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \tag{7}$$

Table 1. Characteristic coefficients of the Lennard-Jones interatomic interactions in the computational force field [17,18]

Particles	σ (Å)	ε (kcal/mol)
	UFF	UFF
H	2.886	0.044
N	3.6660	0.069
Cu	3.495	0.005
Al	4.499	0.505

The computational framework employed ammonia-based refrigerant in conjunction with copper as the operational medium, and they were confined in Al nanochannels a size of 150 × 100 × 100 nm³. The computational domain was configured with invariant spatial constraints along both planar coordinates, while the z-axis direction was set as periodic boundary conditions. A force of 0.02 eV/Å was applied externally to the nanochannel. The simulation was initiated under conditions of 300 K and 1 bar. To maintain structural integrity and accurate temperature regulation, the Nosé-Hoover thermostat was employed. The system was stabilized over a period of 2 ns, with the process assessed by observing temperature and potential energy fluctuations，during which the NVT ensemble was applied. Upon completion of the stabilization process, an additional external electric field was applied to the structure. Figure 1 schematically illustrates the structural model of this simulation study.

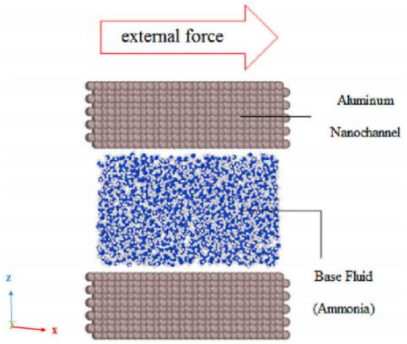

Figure 1. Illustration of applied external forces in the aluminum nanochannel-ammonia refrigerant simulation system

This computational study encompasses following three main stages:

First stage: Examine the structural stability of the atomic configuration in the nanochannel.

Second stage: Evaluate the influence of the electric field on atomic organization and thermal dynamics.

Third stage: Explore the role of nanochannel voids in shaping thermal properties and the behavior of the atomic system during the simulation.

Equilibration Process

In the early stages of simulating ammonia-based fluid flow in nanochannels, the primary is to ensure that the atomic structure under investigation maintains its stability. To accomplish this, the system is initially equilibrated at the target temperature (300 K), with thermal fluctuations in the system being tracked throughout the process. As shown in Figure 2, the temporal evolution of the atomic configuration's temperature during the simulation reveals a gradual convergence toward a steady value. Physically, this equilibration behavior arises from the progressive damping of atomic vibrations within the computational domain as the simulation advances. Specifically, after a period of nanoseconds, the atomic vibrations of the structure under study eventually converge to a level close to 300 K. This temperature stabilization is a result of the movement of particles within the aluminum nanochannel. Given the converging trend of temperature values in the simulation structure, we can infer that there is good compatibility between atomic structure and the force field used in this study. Therefore, over time, the atomic vibrations gradually approach a specific stable value.

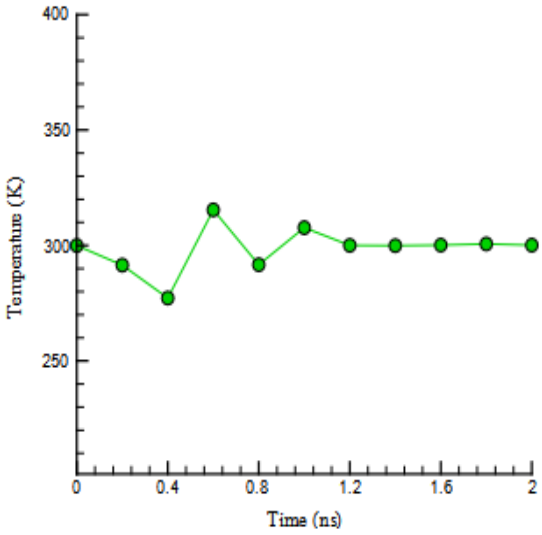

Figure 2. Thermal evolution profile of the simulated atomic configuration

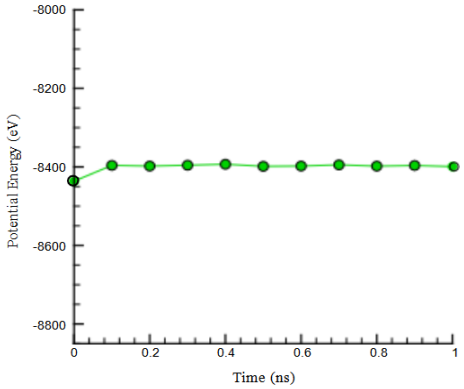

Figure 3. Temporal evolution of potential energy in the simulated system

Another key physical quantity that affects the behavior of structural atoms is the potential energy. Figure 3 shows the changes in potential energy within the sample. As evident from the plot in Figure 3, the interaction energy stabilizes at a final value of -8399.15V. Since the value of the potential energy is negative, this indicates that there is an attractive force between the particles in the atomic structure, which gives the atomic thermal stability. As the value of the potential energy becomes further negative (i.e., more and more negative), the atomic structure in the simulation will exhibit higher. This means that the more negative the potential energy, the more stable the atomic structure, and the more compact and orderly the arrangement of particles within it.

EFFECT OF EXTERNAL

The role of external electric field frequency in modulating atomic-scale structural configurations and thermal characteristics is a critical consideration in simulated systems. To systematically evaluate this phenomenon, our investigation was structured into two domains: structural response and thermal response. For structural analysis, we quantified the correlation between electric field frequency and peak density variation. In thermal analysis, we examined frequency-dependent effects on phase transition kinetics—specifically transition rates, temporal thresholds, and conductive heat transfer. Methodically chosen frequency parameters (0.1, 0.2, 0.3, and 0.51 /ps) were employed to establish comparative frameworks. As depicted in Figure 4, the cross-sectional density profile within the nanochannel exhibits a marginal elevation from 0.028 to 0.03 atoms/Å^3 as frequency escalates from 0.1 to 0.51 /ps. Notably, interfacial interactions between nanoconfining walls and fluidic particles persist as the governing mechanism across all tested frequencies. These dominant interfacial forces effectively stabilize density distribution patterns, rendering frequency-induced modifications statistically negligible within the examined range. This mechanistic dominance substantiates the observed insensitivity of nanofluid density to frequency modulation, confirming its robust equilibrium under variable electric field conditions.

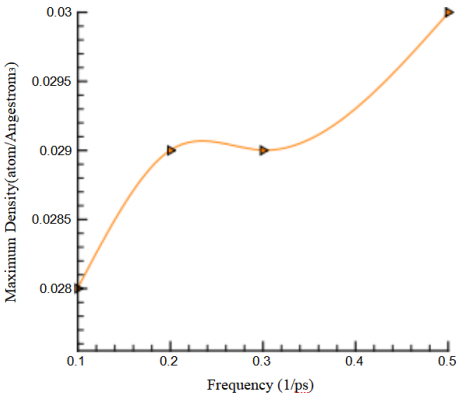

Figure 4. Peak density variations of ammonia-copper nanofluid under applied electric field frequency modulation

Figure 5 demonstrates the frequency-dependent phase transformation kinetics of copper-ammonia nanofluid systems under external electric field modulation. Experimental data reveal a pronounced 49% attenuation in phase transformation efficiency with increasing electric field frequency (0.1-0.51/ps), offering critical insights into the field-regulated nucleation dynamics. Furthermore, spectral analysis indicates a frequency-induced temporal prolongation of the phase transformation process, where

the characteristic transition duration extends from 2.96 ns to 3.0 ns across the tested frequency range. This inverse correlation between excitation frequency and transformation kinetics quantitatively elucidates the relaxation-dominated nature of the phase transition mechanism in charged nanoparticle systems.

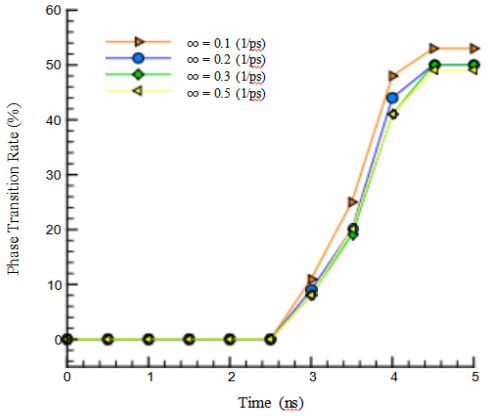

Figure 5. Temporal evolution of phase transition kinetics in ammonia-copper nanofluid system

Experimental results demonstrate that elevated external electric field frequencies induce amplified particle kinetic activity, leading to enhanced stochastic collisions which attenuate thermal transport efficiency in ammonia-copper nanofluids. As shown in Figure 6, the thermal conductivity coefficient approaches stabilization at 0.72 W/m·K when the applied electric field frequency reaches a critical threshold of 0.5 normalized units, indicating a frequency-dependent saturation phenomenon in energy transfer characteristics.

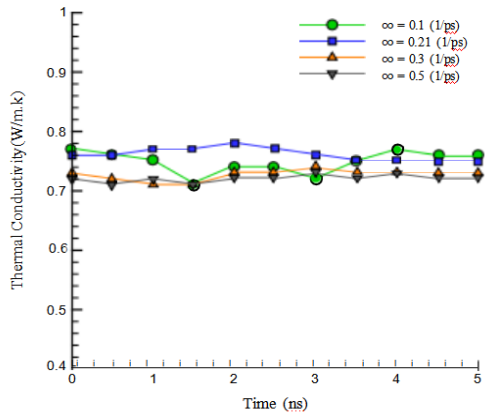

Figure 6. Electric field frequency-dependent thermal conductivity variation in the nanofluid system

Table 2 presents the phase transition characteristics and thermal transport properties of the simulated ammonia-copper nanofluid under varying external electric field frequencies. Notably, at an electric field frequency of 0.51 /ps, the system exhibits a minimum phase transition particle concentration alongside a maximum phase transition duration. This inverse relationship between frequency and thermal efficiency suggests that higher electric field frequencies impair the heat transfer performance of the ammonia-copper nanofluid, highlighting the critical role of field frequency in modulating thermal dynamics.

Table 2. Phase transition characteristics and thermal transport properties under varying electric field frequencies

Electric field frequency (1/ps)	0.1	0.2	0.3	0.5
Phase transition rate (%)	53	50	50	49
Phase change time (ns)	2.96	2.98	3.00	3.00
Thermal conductivity (W/m.K)	0.76	0.75	0.73	0.72

CONCLUSION

Improving the thermodynamic performance of thermal energy exchange systems has become a significant focus for engineers and researchers in contemporary research. This investigation utilizes atomistic modeling approaches to examine thermal transport phenomena of copper nanoparticles within confined nanochannels subjected to external electric field effects. By optimizing the system design, the condensation time of the nanofluids has been significantly reduced. Enhancing the thermal conductivity of nanostructures remains a key objective, with the goal of unlocking their full potential. The results demonstrate that in the simulated atomic systems, the temperature stabilizes at the initial value of 300 K within 2 nanoseconds, while the potential energy reaches equilibrium at -8399.15 eV. Increasing the electric field frequency from 0.11/ps to 0.51/ps extends the relaxation time from 2 to 3 nanoseconds and reduces the thermal conductivity from 0.76 to 0.72 W/mK. Introducing cavities on the nanochannel walls increases the surface contact area, enhancing both atomic interactions and thermal performance. Specifically, the nanochannel with a cubic cavity achieves a peak thermal conductivity of 0.80 W/mK. The phase transition percentages for samples with Hermitic, spherical, and cubic cavities are 65%, 66%, and 68%, respectively. The phase transition times for these samples are 2.88 nanoseconds, 2.87 nanoseconds and 2.85 nanoseconds, respectively. These results provide valuable insights into the optimization of heat transfer systems, highlighting the potential of different cavity shapes and electric field frequencies to enhance the performance of nanofluids in nanochannels.

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REFERENCES

[1] Guo Siyao, Wang Kun, Wang Wenrui, et al. and Application of Binary Eutectic Composite Phase Change Microcapsule Materials. Journal of Composite Materials, 1-8[205-01-03].

[2] Pan Jiajun, Liu Xuran, He Qi, et al. Progress in Cellulose Modification and Enhanced Biodegradable Polymers. Journal of Cellulose Science and Technology, 1-10[202501-03].

[3] Li Zhidong, Han Yue, Huang Lihui, et al. Thermal Characteristics of High-Temperature Organic Phase Change Heat Storage. Guangdong Chemical Industry, 2024, 51 (24): 12-15.

[4] J. Wang, X. Li, Y. Chen, Experimental investigation of R290/R600a mixture as replacement for R134a in domestic refrigerators, Energy Conversion and Management 85 (2014) 591-596.

[5] Wang Y, Jiang L, Cui K, et al. Thermal and textural properties of extruded rice affect its cooking performances and the texture of the steamed extruded rice. Grain & Oil Science and Technology, 2024, 7 (04): 237-245.

[6] An Zhihui, Wu Lei, Li Ruoyao, et al. ystallization behavior, thermal and dielectric properties of PLA composites modified by MXene and PBAT. Plastic Industry, 2024 52 (10): 50-58.

[7] He Yifeng, Li Xiuying, Li Chaoyuan, al. Preparation and characterization of low melting point sealing glass of ZnO-CuO-Bi2O3-B2O3-SiO2 English. Ceramics, 2024, 45 (05): 931-940.

[8] S. Bi, K. Guo, Z. Liu, J. Wu, Performance of a domestic refrigerator using TiO2-R600a nano-refrigerant as working fluid, Energy Conversion and Management 52 (1) (2011) 733-737.

[9] Shan Yuheng, Li An Zhang Xinyu, et al. Effect of matrix thermal properties on laser-induced plasma. Chinese Physics B, 2024, 3 (10): 377-383.

[10] Xiang Haoxuan, Fu Guohong, Yang Tianchun et al. Method for acquisition and processing of dynamic and static information of natural electric fields. Journal of Hunan University of Science and Technology (Natural Science), 2024, 39 (01): 1-10.

[11] S. K. Das, N. Putra, W. Roetzel, Pool boiling characteristics of nano-fluids, International Journal of Heat and Mass Transfer 46 (5) (2003) 851-862.

[12] J. Eapen, W. C. Williams, J. Buongiorno, L. W. Hu, S. Yip, Mean-field versus molecular modeling of the thermal conductivity of nanofluids, Journal of Applied Physics 102 (7) (2007) 074310.

[13] H. Babaei, P. Keblinski, J. M. Khodadadi, Equilibrium molecular dynamics determination of thermal conductivity for multi-component systems, Journal of Applied Physics 112 (5) (2012) 054310.

[14] Y. Xuan, Q. Li, Investigation on convective heat transfer and flow features of nanofluids, Journal of Heat Transfer 125 (1) (2003) 151-155.

[15] P. Keblinski, R. Prasher, J. Eapen, Thermal conductance of nanofluids: Is the controversy over? Journal of Nanoparticle Research 10 (7) (2008) 1089-1097.

[16] Xu Baosheng, Heujie, Fang Daining, et al. Study on carbon fiber composites modified by nanocellulose// Chinese Composite Materials Society, zhou Municipal People's Government. Abstracts of the Third China International Composite Materials Technology Conference - Sessions 6-10. Institute of Solid Mechanics, Tsing University; Beijing Key Laboratory of Lightweight Multifunctional Composite Materials and Structures, Beijing Institute of Technology. 2017: 2.

[17] Dong Sukun, Yuan Qiaolong, Huang Farrong. Performance of silicon-containing arylacetylene resins modified by diaryl diacety propyl ethers// Chinese Composite Materials Society, Hangzhou Municipal People's Government. Abstracts of the Third China International Composite Materials Technology Conference - Sessions1-5. Key Laboratory of Special Functional High Molecular Materials and Related Technologies, Ministry of Education, East China University of Science and Technology. 2011: 1.

[18] Bao H, Meincke T, Taylor KNR. Continuous flow synthesis of metal patchy nanoparticles// National Center for Nanoscience and Technology. China NANO 2013 Abstract Book. Institute of Particle Technology, FAU Erlangen-Nuremberg, Cauerstr. 4, 91058 Erlangen, Germany. 2013: 1.

[19] Bai Shiyu, Zhao Xingyu Lin Jiawei, et al. Study on the relationship between the microstructure of high concentration sodium chloride aqueous solution and the precipitated crystals Journal of Artificial Crystals, 1-10[2025-01-03].

[20] Enji, Hu Siyu, Tan Guangming, et al. Influence and analysis of optimizers on the performance of neural network force fields Computer Science, 1-12[2025-01-03].

[21] Tian Xue, Gong Chaoyun, Yan Fuquan, et al. Mechanism analysis of high pressure combined with natural inhibitors to deactivate polyphenol oxidase based on dynamics simulation. China Fruits and Vegetables, 2024, 44 (12): 13-19.:10. 19590/j. cnki. 1008-1038. 2024. 12. 00.

[22] Wei Zhaozhao. Molecular dynamics simulation of the bending behavior of B2 FeAl alloy nanowires with different orientations. Acta Physica Sinica, 1-31[2025-01-03].

[23] Ni Weixuan, Jia Lixia, Dou Yankun, et al. Atomic-scale simulation study on the creep behavior ofocrystalline molybdenum. Atomic Energy Science and Technology, 1-11[2025-0103].

[24] Xiang Haoxuan, Fu Guohong, Yang Tianchun, et al. for acquisition and processing of dynamic and static information of natural electric fields. Journal of Hunan University of Science and Technology (Natural Science Edition), 224, 39 (01): 1-10.

[25] Huang Xin, He Limin, Luo Xiaoming et al. Study on the mechanism of non-coalescence of two liquid droplets in AC electric field. Journal of Engineering Thermophysics, 022, 43 (05): 1247-1253.

[26] Yang Tao, Wu Xix, Huang Liang, et al. Characteristics of transient radiation electric field during GIS switch operation. Power Big Data, 2021, 4 (10): 53-62.

[27] Yang Qian, Zeng Zhong, Li Jiayu, al. Influence of AC electric field frequency on deformation and fusion of weakly conductive liquid droplets. Journal of Chongqing University, 222, 45 (12): 58-70.

[28] Zhou Jiangang. The relationship between ion concentration and electric field in dielectric barrier discharge. Cryogenics and Special Gases, 2018, 36 (05): 1619.