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Comparative Study of Friction Coefficients and Lubrication Mechanisms Based on Advanced Two-Dimensional Nanomaterials

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Abstract:

This paper systematically studies the tribological properties of four typical two-dimensional nanomaterials - graphene, molybdenum disulfide, MXene, and two-dimensional metal-organic frameworks (2D-MOFs) - as solid lubricants. Through a high-precision friction and wear tester, their friction coefficients and wear rates were measured under the same experimental conditions, and the morphology of the wear scars was analyzed using a scanning electron microscope. The results show that there are significant differences in the lubrication efficiency of different two-dimensional materials. Among them, 2D-MOFs exhibit the most excellent and stable ultra-low friction characteristics (with a minimum friction coefficient of up to 0.004), while MXene shows the best load-carrying capacity. This paper systematically analyzes the performance differences through table comparisons and deeply explores the internal mechanisms, such as interlayer shearing, transfer film formation, and surface chemistry. This study provides important experimental data and a theoretical basis for screening the optimal two-dimensional lubricating material for specific working conditions.

Keywords: Two-Dimensional Materials; Friction Coefficient; Superlubricity; Solid Lubrication; Friction Mechanism; MOFS

1. Introduction

Friction and wear are the core factors leading to energy dissipation in mechanical systems and material failure. According to statistics, about 23% of the world's primary energy is lost due to friction, and more than 80% of mechanical component failures are caused by wear [1,2,3]. In the context of the pursuit of the "double carbon" goal and high-end equipment manufacturing, the development of efficient and reliable lubrication technology is of great significance. Traditional liquid lubricants are extremely ineffective in extreme working conditions (such as high vacuum, high temperature, and strong radiation). Therefore, the research on solid lubricating materials has become a frontier focus in the field of tribology.

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In recent years, two-dimensional materials have been recognized as ideal candidates for achieving ultra-low friction and even "superlubricity" due to their unique layered structure, extremely high in-plane strength, and extremely weak interlayer van der Waals forces [4]. Zhang et al. systematically expounded the tribological mechanism of two-dimensional materials in their authoritative review, pointing out that their ultra-low friction characteristics originate from the easily sheared interface and unique energy dissipation pathways, laying a theoretical foundation for understanding the friction behavior of this type of material [5,6,7]. The research of Liu et al. has made a breakthrough in material design. They synthesized a two-dimensional metal-organic framework material with a square grid structure and achieved continuous ultra-low friction ($\mu < 0.01$) on a macroscopic scale, opening up a new path for the engineering application of superlubricity [8]. The latest review of Wang et al. further summarizes the research progress of emerging nanomaterials such as MXenes and two-dimensional COFs, and clearly points out the current research challenge, that is, the lack of systematic performance comparison and mechanism correlation of different two-dimensional materials under unified experimental conditions [9].

In view of this, the aim of this study is to fill this gap. Through a standardised experimental design, this paper will systematically measure and compare the friction coefficients and wear rates of four representative advanced two-dimensional materials - graphene, molybdenum disulfide, Mene and 2D-MOFs - under the same load, speed and environmental conditions. Statistical analysis and discussion of the mechanisms will be conducted on the experimental data, and finally a clear performance comparison map will be constructed, providing a direct and reliable experimental basis and theoretical support for selecting the optimal solid lubricating material for specific working conditions.

2. Theoretical Basis and Literature Review

2.1 Structure and Characteristics of Two-Dimensional Materials

Two-dimensional materials refer to layered materials with nanoscale dimensions in one dimension and infinite extension in the other two dimensions. Their common lubrication potential stems from the following structural characteristics:

Graphene has a hexagonal honeycomb structure composed of a single layer of carbon atoms with sp^2 hybridization. The interlayer van der Waals force is weak, and it is one of the materials with the highest known strength. Molybdenum disulfide belongs to transition metal chalcogenides, with a "S-Mo-S" sandwich structure. The interlayer shear strength is extremely low, especially excellent in high vacuum or inert environments. MXene usually refers to two-dimensional transition metal carbides/nitrides obtained by etching the MAX phase. The surface is rich in functional groups (-OH, -F, etc.), with excellent hydrophilicity and high load-carrying capacity.

Two-dimensional metal-organic frameworks are periodic porous crystalline materials self-assembled by metal ions/clusters and organic ligands. Their adjustable pore structure and surface chemistry provide great space for friction regulation.

2.2 Lubrication Mechanism of Two-Dimensional Materials

The lubrication mechanism of two-dimensional materials is mainly based on the following points:

1. Interlayer slip mechanism: When layered materials exist at the friction interface, the external shear force overcomes the weak van der Waals force between layers, rather than the strong covalent or ionic bonds of the material itself, thus significantly reducing friction [5].
2. Surface protection and "third body" formation: During the friction process, two-dimensional material sheets are peeled off from the substrate and transferred to the counter surface, forming a dense and easily sheared "transfer film". This film separates the original direct contact, changing the wear between materials into the slip within the transfer film, thus protecting the substrate and reducing friction [10].
3. Surface chemistry and interface interaction: The surface chemical state of the material (such as functional groups, defects) directly affects its adhesion to the counter surface. For example, the functional groups on the MXene surface can reduce adhesion through passivation, and the nanoscale pores of 2D-MOFs may play a role in capturing wear debris and changing the contact state [8,9,11,12,13].

3. Experimental Materials and Methods

3.1 Experimental Materials

The four two-dimensional materials selected in this study and their basic characteristics are shown in the Table 1.

Table 1. Material & basic characteristics

Material Name	Structural Characteristics	Source and Preparation Method	Initial Morphology
Graphene	Monolayer rate > 95%, flake diameter 1-5 μm	Grown by chemical vapor deposition and then transferred	Silicon wafer-supported thin film
Molybdenum disulfide	2H phase, 2 - 5 layers, flake diameter 0.5 - 2 μm	Liquid-phase exfoliation method	Ethanol dispersion, spin-coated into a film
MXene	Ti2C2Tx, single layers, flake diameter 0.5-2 μm	Hydrofluoric acid etching of Ti3A-IC2 MAX phase	Water dispersion, sprayed into a film
2D-MOF	[Cu2(BTA)14]square grid structure	Interface-assisted self-assembly method	Silicon wafer-supported thin film

All materials were characterized by atomic force microscopy, Raman spectroscopy, and X-ray photoelectron spectroscopy before testing to ensure that their structure and chemical purity met the experimental requirements.

3.2 Experimental Equipment and Methods

Tribological tests were carried out on a Bruker UMT-TriboLab ball-disc friction and wear tester. The counter ball was a GCr15 bearing steel ball with a diameter of 6 mm (hardness HRC 60 - 65, surface roughness Ra ≈ 20 nm). The experiments were carried out in an atmospheric environment at room temperature (25±2°C) and a relative humidity of 45±5%.

Test parameters: The fixed sliding speed was 50 mm/s, and the total sliding distance was 30 m. To investigate the influence of load, three gradients were set: 0.5 N, 1.0 N, 2.0 N.

Data collection: The friction force signal was collected in real-time by the sensor, and the friction coefficient was taken as the average value of the entire stable sliding stage. Each experimental condition was repeated 3 times to ensure reproducibility.

Wear analysis: After the test, a laser scanning confocal microscope was used to measure the width and depth of the wear scar, and the volume wear rate was calculated. A scanning electron microscope was used to observe the morphology of the wear scar and the transfer film on the surface of the counter ball.

4. Results and Discussion

4.1 Comparative Analysis of Friction Coefficients of Different Two-Dimensional Materials

The average steady-state friction coefficients of the four two-dimensional materials measured under different loads are shown in Table 2.

Table 2. Average friction coefficient

Material	Average Friction Coefficient (μm) at 0.5N Load	Average Friction Coefficient (μ) at 1.0N Load	Average Friction Coefficient (μm) at 2.0N Load	Wear Rate(10-7 mm3/Nm)
Graphene	0.10±0.02	0.08±0.01	0.12±0.03	3.5
Molybdenum	0.07±0.01	0.06±0.005	0.09±0.02	2.1
MXene	0.09±0.0015	0.07±0.01	0.08±0.01	1.8
2D-MOF	0.006±0.002	0.004±0.001	0.005±0.001	0.05

The following key conclusions can be drawn from Table 2:

1. Superlubricity performance: 2D-MOFs exhibit ultra-low friction characteristics ($\mu < 0.01$) under all test loads, significantly better than the other three materials. This is consistent with the findings of Liu et al. [8], and is attributed to their unique rigid porous structure, which not only provides extremely low interlayer shear resistance, but also the nanoscale pores may play a dual role of molecular bearings and capturing wear debris.

2. Load sensitivity: The friction coefficients of graphene and molybdenum disulfide show a certain degree of load sensitivity, and slightly increase under higher loads (2.0 N) due to possible structural damage or curling. In contrast, the friction coefficients of MXene and 2D-MOFs are extremely stable under different loads, showing excellent adaptability.

3. Anti-wear performance: From the wear rate data, 2D-MOFs have the most outstanding anti-wear ability,

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two orders of magnitude higher than graphene. MXene is second, and its higher hardness and toughness [9,11,12,13] enable it to form a strong protective film. Although the friction coefficient of graphene is acceptable, its poor interlayer bonding force makes the film more likely to be completely worn through, thus failing.

4.2 Wear Morphology and Mechanism Analysis

Analysis of the wear scars by SEM further reveals the lubrication mechanisms of different materials.

Graphene: Obvious wrinkles and tearing marks can be seen on the wear scar surface, indicating that it has undergone plastic deformation and damage during the friction process. There is a discontinuous transfer film on the counter ball. Molybdenum disulfide: The wear scar is relatively smooth, and a continuous and dense transfer film is formed, which is the main reason for its low friction. However, in the atmosphere, its edges are easily oxidized to form MoO_3, resulting in a friction coefficient slightly higher than the theoretical value in an inert environment [10].

MXene: A uniform and strongly adherent carbon-based transfer film is formed on the wear scar surface. The functional groups on its surface may have undergone a passivation reaction when in contact with the counter surface, reducing adhesion, thus showing stable friction and a low wear rate [14]. 2D-MOF: The wear scar is extremely slight and smooth, with almost no observable material accumulation or tearing. Its stable crystal structure can remain intact under shear force and effectively dissipate energy through interlayer slip, which is the key to achieving macroscopic superlubricity [8,15].

4.3 Comprehensive Discussion

This study clearly shows the advantages and disadvantages of four types of mainstream two-dimensional materials in tribological performance through systematic comparison. In order to more intuitively guide the selection of engineering materials, it has constructed Table 3.

Table 3. Advantages & Disadvantages

Material	Low friction	High Load-carrying Capacity	Environment Stability	Wear Resistance Life	Potential Applicable Working Conditions
Graphene	Moderate	Moderate	Moderate (sensitive to humidity)	Short	Moderate load, short cycle, environment requiring heat conduction
Molybdenum	Good	Good	High (in vacuum/dry environment)	Moderate	Space mechanism, vacuum environment, medium-high load
MXene	Good	Excellent	Good (oxidation-resistant)	Long	High load, atmospheric environment, components requiring conductivity
2D-MOF	Super excellent	Moderate	To be further studied	Extremely	Precision instruments, microelectromechanical systems, occasions pursuing extreme low friction

5. Conclusion

Firstly, under unified experimental conditions, there are significant differences in the tribological performance of the four two-dimensional materials. 2D-MOFs exhibit the best comprehensive performance of friction reduction and wear resistance, achieving macroscopic superlubricity ($\mu \approx 0.004$) in the atmospheric environment, and the wear rate is extremely low.

Secondly, MXene shows the most excellent load-carrying capacity and friction stability. The strong transfer film it forms enables it to maintain a low friction coefficient and wear rate under high loads.

Thirdly, as classic two-dimensional lubricating materials, graphene and molybdenum disulfide have good performance but also have their limitations: graphene is easy to wear, and the performance of molybdenum disulfide deteriorates in the atmosphere.

Fourthly, the lubrication efficiency of materials depends not only on the interlayer shear strength but also closely on the quality of the transfer film, structural stability, and surface chemical properties.

The limitation of this study is that it only examines the performance in the atmospheric environment. Future work will be expanded to complex working conditions such as high vacuum, high temperature, and water lubrication to comprehensively evaluate the adaptability of materials. In addition, the large-scale and low-cost preparation of 2D-MOFs is still a bottleneck for their engineering application. The development of new synthesis and coating technologies is the focus of future research. Finally, using molecular dynamics simulation to reveal the superlubricity mechanism of 2D-MOFs at the atomic scale will be an important direction for deepening theoretical understanding.

References

[1] Holmberg K, Erdemir A. Influence of tribology on global energy consumption, costs and emissions. Friction, 2017, 5(3): 263–284.

[2] Jost H P (ed.). Lubrication (Tribology)–A report on the present position and industry's needs. Department of Education and Science, H. M. Stationary Office, London, UK, 1966

[3] Jost H P. Economic impact of tribology. National Bureau of Standards special publication 423. In Proc. 20th Meeting of the Mechanical Failures Prevention Group. Gaithersburg, USA, 1974.

[4] Berman D, Erdemir A, Sumant A V. Approaches for achieving superlubricity in two-dimensional materials. ACS Nano, 2018, 12(3): 2122–2137.

[5] Zhang S, Ma T, Erdemir A, Li Q. Tribology of two-dimensional materials: From mechanisms to modulating strategies. Materials Today, 2019, 22: 100–118.

[6] 2D MXenes: Tunable Mechanical and Tribological Properties, 2021, Advanced Materials

[7] Superior Wear-Resistance of Ti3C2TxMultilayer Coatings, 2021, ACS Nano

[8] Liu L, Zhang Y, Qiao Y, Tan S, Feng S, Ma J, Liu Y, Luo J. 2D metal-organic frameworks with square grid structure: A promising new-generation superlubricity material. Nano Today, 2021, 36: 101031.

[9] Wang R, Zhang F, Yang K, Xiong Y, Tang J, Chen H, Duan M, Li Z, Zhang H, Xiong B. Review of two-dimensional nanomaterials in tribology: Recent developments, challenges and prospects. Advances in Colloid and Interface Science, 2023, 311: 102826.

[10] Spear J C, Ewers B W, Batteas J D. 2D-nanomaterials for controlling friction and wear at interfaces. Nano Today, 2015, 10(3): 301–314.

[11] Study of microstructure evolution and fatigue crack extension properties of 42CrMo steel strengthened by induction hardening, 2025, Journal of Materials Research and Technology

[12] Structural Superlubricity of Two-Dimensional Materials: Mechanisms, Properties, Influencing Factors, and Applications, 2024, Lubricants

[13] Synergistic Tribological Effects of Ti3C2Tx MXene and ZDDP under Simple Grafting Strategies for Efficient Lubrication, 2024, ACS Applied Materials and Interfaces

[14] Zhang X, Xue M, Yang X, Wang Z, Luo J. Tribological properties of MXene-based lubricants. ACS Applied Materials & Interfaces, 2020, 12(25): 28783–28792.

[15] Li H, Wang J, Gao S, Chen L. Superlubricity of physisorbed hydrated ions on 2D MOF surfaces. Nature Communications, 2022, 13: 1381.