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Investigating the Properties and Applications of Hydrophobic Materials: The Case of Polydimethylsiloxane (PDMS)

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Abstract. For materials with different functions, their surface properties have different requirements. Among them, the hydrophobic property plays an important role in various fields such as anti-fouling, industrial production, microfluidics, and anti-icing. During the research process, it was discovered that many structures of plants and animals in nature have excellent hydrophobic functions, such as the self-cleaning property of the lotus leaf surface and the sticky superhydrophobic property of the surface of rose petals. Moreover, their mechanisms can be imitated and utilized. Based on the basic characteristics of surface properties, this paper takes the good base material polydimethylsiloxane (PDMS) as an example to study the performance of the hydrophobic material combined with silica, and the results confirmed by infrared spectroscopy show that the introduction of target functional groups and the contact angle and rolling angle conform to the results of superhydrophobic properties. This research result provides an efficient and green synthesis idea for superhydrophobic research and is beneficial to the development of hydrophobic materials.

Keywords: Hydrophobicity, Surface behavior, Bionics, Composite materials

1. Introduction

Materials with hydrophobic properties have extensive applications in various fields of life and industrial production, leading to significant breakthroughs in areas such as marine anti-fouling, biological antibacterial, and building materials. For instance, researchers utilized the stearic acid structure on the surface of lotus leaves and combined zinc stearate with volcanic ash to prepare cement additives [1]. These additives have shown remarkable effects in waterproofing and extending the lifespan of materials. Based on the hydrophobic mechanisms of different plants and animals in nature, such as the microstructure of papillae on the surface of lotus leaves, the main indicators for measuring the hydrophobic properties of materials were obtained, including the range of rolling angle and contact angle, and surface roughness. Polydimethylsiloxane (PDMS), with its good chemical stability and special molecular structure, is currently one of the main base materials for composite hydrophobic materials. This paper explores the performance of composite materials with PDMS as the base in fabricating hydrophobic coatings. The results are demonstrated by infrared spectroscopy, contact angle, and rolling angle, etc., showing their performance. The preparation of

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this coating material has certain contributions and inspirations for areas such as drainage and food preservation, and also provides ideas for the optimization of other biomimetic hydrophobic materials.

2. Surface behaviors existing in nature

The earliest record of lotus leaf self-cleaning can be traced to Tao Yuanming's phrase "not tainted by the mud." Later, Barthlott and Neinhuis used scanning electron microscopy (SEM) to reveal the micrometer-sized papillae and nanometer-waxy crystal hierarchical structure on lotus leaf surfaces, officially naming the "lotus leaf effect." Subsequently, many other organisms were found to exhibit hydrophobic behaviors, though via different mechanisms—rice leaves rely on surface anisotropy, while water striders utilize an air film. Inspired by these natural examples, various functional materials have been developed. For instance, cactus spines feature gradient grooves and barbs that enable fog collection. The barbs capture water droplets, and the spine structure creates a Laplace pressure difference from tip to base, driving droplet movement. This unique design shows great potential for water collection applications [2].

As shown in Figure 1, the lotus leaf's self-cleaning hydrophobicity arises from its two-layer hierarchical rough structure: micrometer-sized protuberances (5–10 μm in diameter) and nanometer-sized wax crystals (~100 nm in diameter). The protuberances create numerous gaps that trap air, significantly reducing the contact area between water molecules and the leaf surface. The wax crystals, composed mainly of long-chain fatty acid esters and alkanes, possess a much lower surface energy than water, hindering water adhesion. The combined effect of these two structures produces the famous "lotus leaf effect." This superhydrophobic and self-cleaning mechanism is now widely applied in waterproof outerwear, mechanical equipment maintenance, and marine anti-fouling for ships [3].

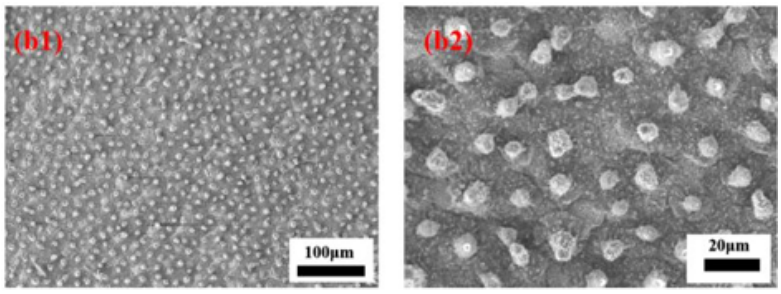


Figure 1. SEM image of the surface structure of lotus leaves [4]

3. Hydrophobicity evaluation indicators

3.1. Contact angle

Generally, the angle formed by the tangent of the liquid-gas interface at the junction of the solid, liquid, and gas phases and the solid-liquid interface is called the contact angle, denoted by θ. The size of θ can directly reflect the degree of hydrophobicity, that is, the smaller the contact angle θ, the easier the liquid spreads on the solid surface, and the hydrophilicity and wettability are good; the larger θ is, the less easy the liquid is to spread on the solid surface, and the hydrophobicity is good while the wettability is poor. Hydrophilicity usually refers to the tendency of the liquid to spread on the solid surface due to the interaction between the liquid and the solid surface, while hydrophobicity refers to the tendency of the liquid to form a spherical shape on the solid surface due

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to the interaction between the liquid and the solid surface. According to the size of θ, materials are usually classified into three categories. Materials with hydrophilic properties have a contact angle θ < 90°, and the liquid can wet a certain area on their surface; materials with hydrophobic properties have a contact angle between 90° < θ < 150°, while those with θ > 150° are superhydrophobic [5].

3.2. Young's equation and contact lag theory

Thomas Young and Laplace proposed Young's equation, which was the first to discuss the relationship between the contact angle at the interface and surface tension from the perspective of energy:

$$\gamma_{SG} = \gamma_{SL} + \gamma_{LG}\cos\theta \tag{1}$$

Here, γ_{SG}, γ_{SL}, and γ_{LG} represent the surface tensions of solid-gas, solid-liquid, and liquid-gas, respectively. This equation explains the relationship between the contact angle and the interfacial tension, but it can only be satisfied under a relatively ideal state. The contact lag theory, on the other hand, can more realistically reflect the actual situation. The contact angle lag is generally expressed as:

$$\Delta\theta = \theta_a - \theta_r \tag{2}$$

That is, the difference between the maximum contact angle when the liquid expands and the minimum contact angle when the liquid contracts. When $\Delta\theta$ is small, the liquid is less likely to adhere to the solid surface, while the opposite is true when the liquid has a higher adhesion. Usually, materials with a contact angle $\theta > 150°$ and a contact angle lag $\Delta\theta < 10°$ are classified as superhydrophobic materials. In addition, factors such as surface roughness and geometric configuration, which affect the hydrophobic properties, are also multiple factors that form the basis of the study of hydrophobic materials [6].

4. Represented by a typical hydrophobic coating matrix material - polydimethylsiloxane

4.1. Basic structure of polydimethylsiloxane

The hydrophobic property of the material largely stems from the functional groups it carries, such as the large amount of stearic acid（$-C_{17}H_{35}$）on the surface of lotus leaves. Polydimethylsiloxane (PDMS), as a widely used raw material for the preparation of superhydrophobic material matrices and coatings at present, has hydrophobic methyl groups on its side chains（$-CH_3$）. Moreover, PDMS itself has a very low surface tension, high surface activity, and hydrophobicity, and these properties are closely related to its chain structure. The large number of $Si-O-Si$ in the PDMS structure has a longer bond length and a larger bond angle, thus making the molecular chain relatively soft and causing the methyl groups on the side chains to face outward from the main chain, forming a low surface energy, non-polar hydrophobic layer.

4.2. Preparation of PDMS-SiO_2 composite hydrophobic coating by doping SiO_2 nanoparticles with PDMS as the matrix

First, nano-sized SiO_2 particles were synthesized using tetraethyl orthosilicate (TEOS) as the raw material. The ethoxy and silicon-oxygen bonds in TEOS undergo hydrolysis under suitable conditions, producing $Si(OH)_4$. This product further condenses with TEOS to form unstable nuclei, which then aggregate and grow. Due to strong repulsive forces between particles, they eventually disperse into stable SiO_2 nanoparticles. The reaction was catalyzed by ammonia water in anhydrous ethanol, and after centrifugation and stirring, the white precipitate of SiO_2 nanoparticles was obtained. However, the as-prepared SiO_2 surfaces still carry many hydrophilic groups (e.g., free

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hydroxyls), which would interfere with hydrophobic coating formation. Therefore, a silane coupling agent containing hydrophobic groups, specifically dodecyl trimethoxysilane (DTMS), was used. Upon hydrolysis, the silane coupling agent generates Si–OH that reacts with surface hydroxyls to form the target Si–O–Si bonds, rendering the nanoparticles hydrophobic [7].

Second, the hydrophobic SiO_2 nanoparticles were dispersed in ethyl acetate to prepare a SiO_2 dispersion. This dispersion was mixed with the PDMS polymer under magnetic stirring until a uniform suspension was obtained. The PDMS-SiO_2 suspension was then applied onto substrates such as glass and allowed to cure completely, yielding the final hydrophobic composite coating.

4.3. Result testing and analysis

4.3.1. Infrared spectrum

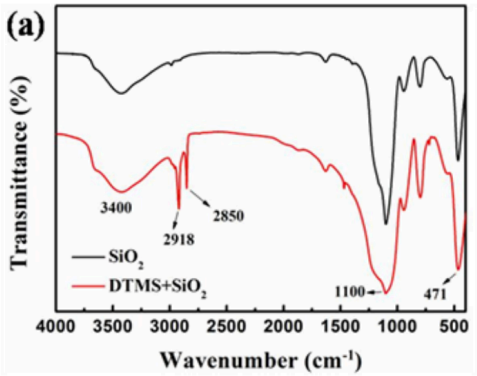


Figure 2. Infrared spectrum of composite materials

As shown in Figure 2, the red spectrum represents the spectrum after DTMS modification. At positions 2918 cm^{-1} and 2850 cm^{-1}, there are two additional absorption peaks compared to the spectrum before modification. This is caused by the symmetrical stretching of $-CH_3$ and the asymmetrical stretching of $-CH_2-$, which successfully proves that the functional groups of DTMS have been transferred to the nanoparticles after modification. At 471 cm^{-1} before and after modification, the peak is caused by the vibration of $Si-O-Si$, which also successfully proves its introduction.

4.3.2. Contact angle and rolling angle

PDMS is used as the base material, and SiO_2 is used as the key additive to achieve hydrophobic properties. In the evaluation, the diameter of SiO_2 particles and their addition amount are taken as variables, and the rolling angle and contact angle are observed. During the test, water droplets were added to the PDMS surface without SiO_2 particles, and the contact angle was approximately 110°, which met the conditions for hydrophobicity; in terms of the rolling angle, due to the high viscosity, there was no rolling angle. When adding SiO_2 nanoparticles, when the mass ratio of nanoparticles to the base material reached approximately 0.8, the contact angle exceeded 150°, and the rolling angle was only about 2.4°, which is a relatively ideal superhydrophobic state. However, when the amount of nanoparticles was further increased, the contact angle decreased, and the hydrophobic performance deteriorated. It is speculated that this might be related to the excessive SiO_2 causing the disruption of the internal stress balance and the destruction of the structure in the system.

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5. Applications of PDMS in practice

The research on antibacterial properties is an important topic in combating pollution at present. Among them, the hydrophobic material surface serves as a key link, which can reduce water residue and inhibit the growth and reproduction of bacteria. Shim et al. studied a dual-hydrophobic and photocatalytic antibacterial film, combining photocatalytic activity with hydrophobicity. PDMS, due to its excellent smooth and hydrophobic surface that can reduce bacterial adhesion, is used as the base. Tetra butylammonium (TBA) is inserted into the layered titanate, and the photocatalytic performance is enhanced by synthesizing tetra butylammonium interlayer titanates. After exposure to sunlight, the removal efficiency of methylene blue reached 53.9%, and its antibacterial tests on Escherichia coli and Staphylococcus aureus confirmed the bactericidal activity and proliferation inhibition. The results show that this antibacterial material has significant potential when combined with PDMS [8].

The inherent hydrophobicity of PDMS can be modified. Its excellent intrinsic permeability enables it to be widely used in selective permeable membranes. Surface modification under specific conditions can impart hydrophilicity. Shi et al. constructed a polymer interpenetrating network on the PDMS surface. The difference between the aqueous phase and the organic phase allowed low-molecular-weight hydrophilic polyethyleneimine (PEI) to penetrate PDMS and undergo a cross-linking reaction with the organic phase. PEI was fixed on the PDMS surface, ensuring permeability while enhancing hydrophilicity [9].

6. Discussion

Nanohydrophobic materials, as a highly promising research field at present, are mostly obtained by modifying the base materials to achieve the target performance. As one of the most widely applied base materials, PDMS has excellent mechanical properties, good hydrophobicity by itself, and stable chemical properties. However, PDMS also has some drawbacks that are detrimental to the material's performance. For example, Yao et al. found in the mechanical performance experiments of nanomaterials with PDMS as the base material that other mechanical properties, such as hardness and modulus, showed temperature sensitivity, and the modulus of the surface-dominated mechanical response decreased particularly significantly at high temperatures, confirming that the coating was sensitive to temperature [10]. Moreover, as mentioned in the previous discussion on the composite materials with SiO_2 polymerization, its compatibility with non-polymeric materials is poor, and the agglomeration is poor. And silicon, titanium, etc., are commonly used fillers, so this defect also needs to be improved. In conclusion, PDMS is still a base material with great potential in surface performance and has a very wide application field.

7. Conclusion

The main objective of the research is to combine the biological hydrophobic properties and explore a biomimetic hydrophobic composite material with excellent mechanical properties and durability. The surface of a lotus leaf has papillary structures and a waxy layer, and it is modified with low surface energy compounds similar to the chemical composition of the waxy layer, providing a design idea for hydrophobic materials. The research results offer a feasible synthesis approach for the study of superhydrophobic biomimetic nanomaterials, and have a promoting effect on the development of research on hydrophobic materials in daily life and surface performance. In the analysis of the experimental results, the wear resistance of the synthesized composite material

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decreases under a large pressure, which may be related to the performance of the product or the randomness of the test. In future research on hydrophobic materials, the characterization of performance should be more diverse and universal. The development of future hydrophobic biomimetic materials will also make a significant contribution to technological life.

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