Atomic-Scale Modulation of Surface Roughness for Tunable Wettability in Bio-Inspired Nanostructures

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Abstract

Atomic-scale modulation of surface roughness offers a precise and programmable approach to controlling wettability across bio-inspired nanostructures. This study presents a multiscale fabrication strategy integrating strain-induced patterning with nanoscale deposition to achieve tunable contact angles ranging from hydrophilic to superhydrophobic regimes. Wettability transitions were systematically evaluated through surface profilometry, contact angle hysteresis analysis, and adaptive cycle testing. Hierarchical geometries inspired by lotus leaves and spider silk enabled directional water transport and selective adhesion functionalities, with implications for fog harvesting, biosensing, and lab-on-chip platforms. The results demonstrate that atomic-level roughness not only expands the tunable range of surface energy states but also enhances mechanical durability under cyclic strain. The study contributes to next-generation surface engineering by proposing a scalable framework for wettability control via nanogeometric reconfiguration.

Keywords

Atomic-scale roughness, Tunable wettability, Bio-inspired nanostructures, Surface engineering, Contact angle hysteresis, Hierarchical topographies, Strain-induced patterning, Adaptive coatings, Water transport, Nanoarchitectonics

1. Introduction

Nature offers a compelling blueprint for surface functionality through the intricate modulation of wettability observed in biological structures such as lotus leaves, beetle shells, and spider silk. These systems achieve adaptive water repellency, directional transport, and self-cleaning via hierarchical architectures that manipulate surface energy at both micro and nano scales. Translating such capabilities into engineered materials demands precise control over roughness parameters at the atomic level.

Recent advances in nanoscale fabrication, including strain-induced patterning, chemical vapor deposition (CVD), and femtosecond laser texturing, have enabled the design of bio-inspired surfaces with tunable wettability profiles. Unlike conventional approaches that rely on static surface chemistries, atomic-scale roughness modulation allows dynamic reconfiguration of contact angles in response to external stimuli, thereby expanding the operational envelope of smart surfaces.

This study investigates the relationship between atomic-level roughness gradients and wettability transitions, integrating multiscale design principles with functional testing under cyclic strain. By mimicking natural systems and evaluating engineered analogues through contact angle hysteresis, adhesion metrics, and water transport analysis, the research aims to establish a neutral and scalable framework for adaptive surface engineering. The findings carry relevance across fields ranging from

biosensing and fog harvesting to lab-on-chip technologies, where controllable interfacial dynamics are critical.

2. Materials and Methods

2.1 Substrate Preparation and Nanostructure Fabrication

Silicon and molybdenum disulfide (MoS_2) wafers were selected as substrates due to their high surface stability and compatibility with nanostructuring processes. Prior to fabrication, substrates were ultrasonically cleaned in acetone, ethanol, and deionized water, followed by nitrogen drying. Atomic-scale surface features were engineered using a combination of:

Strain-Induced Patterning: Mechanical strain was applied via controlled substrate bending to generate nanoscale stress fields conducive to topographical reconfiguration.

Chemical Vapor Deposition (CVD): Deposition of hydrophobic coatings was achieved using hexamethyldisilazane (HMDS) in a low-pressure chamber at 150°C.

Femtosecond Laser Ablation: High-precision pulse shaping was employed for hierarchical structuring with spatial resolution below 100 nm.

2.2 Surface Roughness and Morphological Characterization

Atomic force microscopy (AFM) was used to quantify surface roughness parameters, including root mean square (RMS) height and asperity distribution. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) provided high-resolution imaging of nanostructure morphology and layering interfaces. Surface energy was inferred via X-ray photoelectron spectroscopy (XPS) analysis.

2.3 Wettability Assessment

Contact angle measurements were performed using a goniometer at room temperature with 5 µL DI water droplets. Each sample underwent:

Static Contact Angle Evaluation

Contact Angle Hysteresis: Advancing and receding angles were calculated to determine surface adhesion characteristics

Cycle Durability Testing: Wettability response was recorded over 1000 strain-release cycles to evaluate reconfigurability and mechanical stability.

2.4 Bio-Inspired Architecture Design

Nanogeometries were modeled based on natural analogues (e.g. spider silk dragline profiles and lotus leaf microtopographies), with directional transport simulated via finite element analysis. The translation of biological patterns into synthetic architectures followed neutral, parametric optimization protocols to ensure reproducibility.

3. Results

3.1 Surface Roughness Modulation and Morphology

Atomic force microscopy (AFM) revealed RMS roughness values tunable between 1.8 nm and 14.3 nm across differently patterned substrates. Femtosecond laser structuring produced nanoasperities with lateral dimensions below 90 nm, forming dual-scale topographies that resembled natural cuticular features. SEM imaging confirmed consistent distribution of hierarchical nanoflowers on MoS_2 substrates, while strain-induced patterns yielded reversible wrinkle-like geometries under cyclic loading.

3.2 Wettability Transitions and Contact Angle Dynamics

Contact angle measurements showed a progressive shift from hydrophilic (≈83° ± 2°) to superhydrophobic states (≈156° ± 1.5°) corresponding to increasing surface roughness. Hysteresis values dropped below 6° in optimized topographies, indicating minimal adhesion and efficient water droplet mobility. Dynamic cycling over 1000 strain-release events maintained wettability stability with <3% deviation, highlighting mechanical resilience of the roughness gradients.

3.3 Bio-Inspired Transport and Adhesion Control

Finite element simulations confirmed directional water migration along dragline-mimetic nanoridges. Experimental fog harvesting trials demonstrated 22–34% increase in water capture efficiency relative to unpatterned controls. Drop adhesion tests revealed anisotropic transport consistent with natural analogues, achieving controlled pinning and release under lateral motion.

3.4 Comparative Analysis with Natural Surfaces

A benchmarking matrix (Table 1) compared engineered surfaces with biological references, quantifying overlap in topographic fidelity, contact angle range, and transport behavior. The lotus-leaf analogue achieved the highest wettability modulation, while spider silk-mimetic substrates exhibited superior directional control under low humidity.

Table 1. Comparative Benchmarking of Bio-Inspired vs Engineered Surface Topographies

Surface Type	RMS Roughness (nm)	Contact Angle Range (°)	Adhesion Behavior	Directional Transport	Structural Fidelity (%)
Lotus Leaf (natural)	~12.5	140–155	Low hysteresis (<5°)	Passive droplet roll-off	Baseline (100%)
Spider Silk (natural)	~8.7	110–135	Anisotropic adhesion	Capillary-guided motion	100%
Engineered MoS$_2$ Surface	14.3	156 ± 1.5	Minimal adhesion (<6°)	Enhanced fog channeling	92.4%
Strained Si Substrate	10.2	83–142	Reversible adhesion modes	Controlled ridge flow	88.7%
CVD-Coated Hybrid Surface	9.8	120–150	Moderate hysteresis	Isotropic wetting	85.1%

The **Structural Fidelity** column estimates design correlation with natural analogues based on topographic profile mapping, adhesion metrics, and water transport behavior

4. Discussion

The data presented in this study confirms that atomic-scale modulation of surface roughness offers a robust pathway for achieving tunable wettability across a wide functional range. The observed transition from hydrophilic to superhydrophobic states — governed by nanogeometric structuring and strain-responsive topographies — aligns closely with biological precedents while establishing distinct advantages in mechanical durability and reconfigurability.

4.1 Comparative Relevance to Natural Analogues

Engineered surfaces modeled after lotus leaves and spider silk not only replicated directional water migration and low hysteresis properties, but also demonstrated greater endurance under cyclic strain. This suggests that synthetic translation of bio-inspired architectures can preserve desirable interfacial

traits while extending operational stability. The fidelity metrics (Table 1) support the notion that atomic-scale design achieves near-parallel behavior across wetting regimes.

4.2 Implications for Smart Surface Applications

The ability to reversibly tune wettability and adhesion presents opportunities for dynamic coatings, fog harvesting systems, and microfluidic device interfaces. Directional transport and adaptive wetting could be leveraged in biosensor surfaces requiring selective fluid motion or minimal fouling. Additionally, the reconfigurability observed under mechanical strain could inform surface designs for wearable systems or responsive textiles.

4.3 Limitations and Prospects for Further Development

While this study achieved stability across 1000 strain cycles, long-term environmental exposure, thermal cycling, and multi-fluid testing remain critical for assessing real-world durability. Furthermore, the fabrication techniques — particularly femtosecond ablation and strain-induced patterning — require optimization for large-area scalability without loss of nanogeometric precision.

Future research may explore hybrid structuring approaches that integrate atomic-scale roughness with surface chemical modulation, potentially expanding wettability control into stimuli-responsive domains (e.g. pH or ionic strength). The incorporation of simulation-informed geometric models could also enable predictive tuning of fluid dynamics across varying biomimetic surface designs.

5. Conclusion

This study establishes that atomic-scale modulation of surface roughness provides a reliable and programmable framework for achieving tunable wettability in bio-inspired nanostructures. By integrating hierarchical topographies with strain-responsive fabrication, surfaces were engineered to mimic and, in some metrics, outperform natural analogues in contact angle range, droplet transport efficiency, and mechanical resilience.

The findings underscore the utility of multiscale design in expanding functional control over interfacial phenomena, particularly in applications demanding adaptive wetting behavior. Through methodical characterization and comparative benchmarking, the research demonstrates the viability of replicating directional water migration, low adhesion, and surface reconfigurability using neutral, scalable techniques.

Future directions may explore the integration of chemical stimuli with atomic-scale roughness to enable multi-modal responsiveness, as well as the translation of these architectures into deployable platforms for environmental sensing, biomedical interfaces, and energy-harvesting materials. This contribution lays foundational insight for the next phase of smart surface engineering rooted in biomimetic fidelity and atomic precision.

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