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Molecular Dynamics Optimization of OTS Coatings and Implications for High-Precision Atomic Magnetometry

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Molecular Dynamics Optimization of Multilayer OTS SAMs Cells for Enhanced Performance in Single Beam SERF Magnetometers

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The development of high-performance octadecyltrichlorosilane (OTS) SAMs is crucial for mitigating alkali-metal spin relaxation and enhancing the sensitivity of spin-exchange relaxation-free (SERF) magnetometers. In this work, we employ molecular dynamics (MD) simulations to investigate the structural, interfacial, and dynamical properties of OTS SAMs, focusing on optimizing their anti-relaxation behavior. By systematically tuning key simulation parameters, including adsorption energy, wettability, and atomic interaction dynamics. Our findings provide a comprehensive framework for the rational design and optimization of OTS SAMs, paving the way for next-generation atomic magnetometers with enhanced stability and prolonged coherence times. Furthermore, we discuss the broader implications of these advancements in quantum sensing and precision measurement applications.

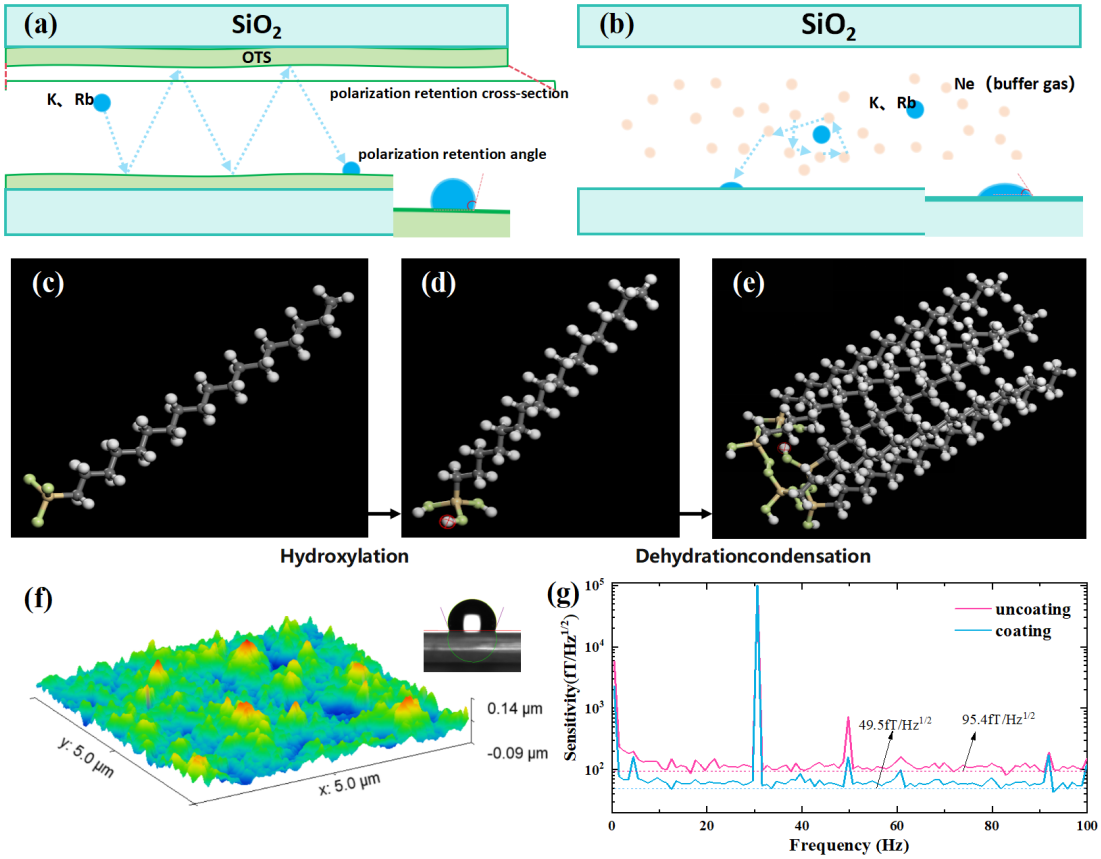

Figure 1: (a) Relaxtion of coating cell, (b) relaxation of uncoating buffer gas cell,the molecular cross linking process of OTS : hydroxylation(c to d) and dehydration condensation(d to e), (f) AFM and contact angle test of OTS SAMs, (g) sensitivity of coating and uncoating magnetometer

References

(1) Xu Y, Pei H, Cong Y, et al. A non-thermal method to maintain alkali vapor density of anti-relaxation coating cell in spin exchange relaxation-free magnetometer[J]. Measurement, 2025, 242: 115960.

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