In situ Thermal Degradation of Monolayer MoS_2 in Oxygen

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Abstract

Monolayer MoS_2 is a key two-dimensional semiconductor for electronic and catalytic applications, where thermal and environmental stability directly impact device performance and reliability.[1,2] Long-time exposure of MoS_2 flakes to ambient air has been shown to induce gradual oxidation that initiates from the edges toward the interior of MoS_2.[3] Under thermal treatment in air, anisotropic etching of monolayer and few layers MoS_2 occurs, often initiating across the basal plane in triangular morphologies.[4] When grain boundaries are present, thermal degradation can originate from interior regions near these boundaries rather than exclusively from the edges.[3] The resulting etching patterns vary considerably depending on experimental conditions and sample qualities. It has been proposed that oxygen induced thermal degradation proceeds through the reaction between O_2 and MoS_2 to form volatile MoO_3 and gaseous SO_2.[5,6] However, these gaseous products are difficult to directly detect, and unambiguous experimental evidence for their formation during etching remains limited.[7] The detailed reaction mechanism governing oxidative thermal degradation is still not fully understood. In this work, we employ in situ variable temperature Raman microscopy to systematically investigate the thermal stability and oxygen reactivity of monolayer MoS_2 under controlled atmospheres. The kinetics of thermal degradation in monolayer MoS_2 flakes are found to proceed through a 2-stage process that depends strongly on both annealing temperature and environmental oxygen concentration. In addition to previously reported morphologies, we observe a distinct etching pattern that initiates within the interior of the flake and propagates outward. These results provide direct spectroscopic and microscopic insight into oxygen driven thermal degradation while demonstrating variable temperature Raman spectroscopy to be a sensitive approach for monitoring structural evolution during oxidative etching.

References

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