Effects of Strain and Local Topography on Electromechanical Coupling in Monolayer Transition Metal Dichalcogenides

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Two-dimensional transition metal dichalcogenides (2D TMDs) have been extensively studied in recent years due to their remarkable electronic, optical, and mechanical properties. Their ability to withstand high levels of strain without fracture makes 2D TMDs attractive candidate materials for devices such as quantum emitters and energy harvesters. However, the high sensitivity of 2D material properties to nanoscale morphology and strain can just as easily interfere with as aid in optimal device performance if not fully understood and accounted for. In this work, we use piezoresponse force microscopy (PFM) to demonstrate that nanobubbles present in exfoliated MoS_2 monolayers significantly alter the electromechanical behavior of these samples and exhibit strong out-of-plane PFM responses due to flexoelectricity. Small bubbles with diameters under 100 nm consistently exhibit enhanced piezoresponse compared to flat regions. Without filtering images for these ubiquitous features, effective piezoelectric coefficients based on PFM of exfoliated monolayer MoS_2 will be systematically overestimated. Large bubbles with diameters on the order of hundreds of nanometers present an even more remarkable pattern. Rather than increasing monotonically from perimeter to apex, the piezoresponse amplitude of large bubbles reaches its peak at the perimeter and subsequently decreases toward a local minimum at the bubble apex. This profile can be correlated with the curvature of the bubble topography, which is related to the local strain gradient. These correlations suggest a link between local electromechanical properties and strain gradients present in these regions. We argue that the large strain gradients at the bubble edges induce a local reduction in spatial symmetry, which produces out-of-plane polarizations via the flexoelectric effect. On subsequent characterization using PFM, these regions effectively behave not as a 2H MoS_2 monolayer, but as a low-symmetry material exhibiting out-of-plane piezoelectricity.

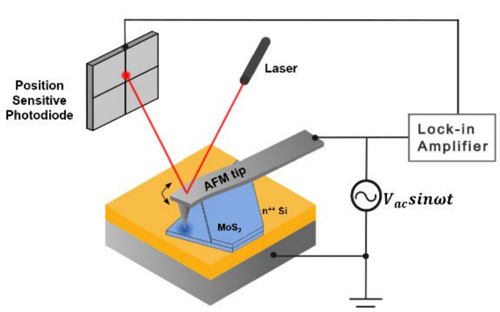

Figure 1. Schematic of PFM measurement setup.

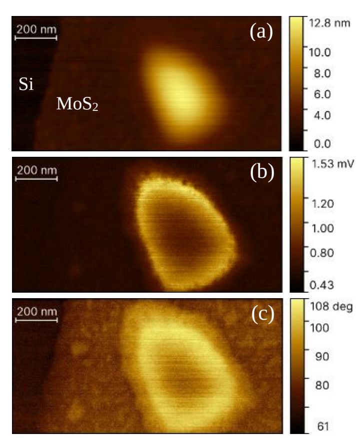

Figure 2. PFM (a) topography, (b) amplitude, and (c) phase of a large bubble in monolayer MoS_2 on n^{++} Si.