

Structural characterization of single layer $V_{1+x}S_2$ on Au (111)

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Vanadium disulphide (VS_2) distinguish itself among other single layer (SL) transition metal dichalcogenides (TMDCs), by having theoretically predicted magnetic properties which can be important for future spintronic and data storage devices [1]. This material is currently understudied as both SL and bulk VS_2 are challenging to synthesize. While the stoichiometric bulk VS_2 is thermodynamically metastable, the SL is unstable in air and requires preparation under vacuum conditions.

Here we report the growth of high-quality SL VS_2 in the octahedral (1T) structure, prepared epitaxially on a Au (111) substrate under ultra-high vacuum (UHV) conditions. During the initial stages of growth, the SL has well-defined triangular islands. At higher coverage, the SL exhibits the typical hexagonal moiré structure observed for other SL TMDCs grown on the (111) face of Au [2]. When the sample is annealed to 400°C in UHV, we observe a transition to a sulphur-depleted phase characterized by a distorted hexagonal unit cell. With higher temperature (550°C) annealing, further sulphur depletion leads to an entirely new SL crystal structure. This last phase has a rectangular unit cell that has not been previously reported for either the bulk or SL forms.

By means of scanning tunnelling microscopy, low-energy electron diffraction, and X-ray photoelectron diffraction, we elucidate the structural properties of both the stoichiometric and sulphur-depleted SL compounds.

[1] M. Kan, B. Wang, Y. H. Lee, and Q. Sun, *Nano Research* 8, 1348 (2015)

[2] S. S. Grønberg, S. Ulstrup, M. Bianchi, M. Dendzik, C. E. Sanders, J. V. Lauritsen, P. Hofmann, and J. A. Miwa, *Langmuir*, 2015, 31 (35), pp 9700–9706