The Effect of CVD Growth Configuration on the stability of MoS_2

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Two-dimensional (2D) transition metal dichalcogenide (TMD) semiconductors (MoS_2, WS_2, and $MoSe_2$ etc.) have appealed significant attention because of their exclusive mechanical, electrical and optical properties. In particular, MoS_2 is one the most popular member of this TMD family as a potential candidate for next generation electronic and optoelectronic devices such as phototransistors, biosensors and photodetectors [2]. In addition to the investigation of the performance of MoS_2 as an active material in device applications, the research on its long term physical stability is also of particular importance for stable device performance. Recent studies show that the chemical vapor deposition (CVD) grown TMD monolayers are not physically stable under ambient conditions [1]. Here, we provides a solution for the stability and fracture formation problems of TMDs (specifically, of MoS_2 monolayers) by proposing a favorable CVD growth geometry that provides the control of the precursor vapor concentration on the growth surface. In this study, the long-term stability of two different growth configurations which are face-down (FD) (commonly used) and horizontal (HO) (proposed) are investigated by keeping the remaining parameters identical. The stability of the grown structures are examined by long term observation and thermal aging experiments Along with these, the first principle calculations are employed to understand the mechanism of cracking behavior for different defect and stress conditions. It is shown that naturally (18 months) and thermally aged MoS_2 monolayer flakes grown by HO (proposed) configuration, retain their stability (Fig 1.c and 1.d) while FD-grown (commonly used) ones lose their structural integrity by formation of cracks and fractures (Fig 1.a, 1.b, 1.e and 1.f). Our results of DFT simulations suggest that the S-vacancies are critical on crack formation thus needs to be avoided for oxidation resistant monolayers. Hence, DFT simulations, time dependent observations and thermal aging experiments show that stability of 2D MoS_2 flakes can be controlled by CVD growth configuration.

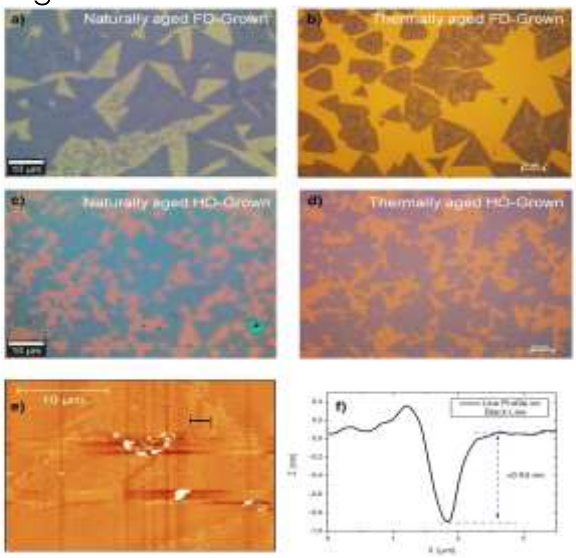

Figure 1: Optical microscope images of 18 month naturally aged FD grown (a) and HO-grown (b) MoS_2 flakes, thermally aged FD grown (c) and HO-grown (d). The AFM image of thermally aged and cracked FD grown MoS2 flake (e) and line profile on black line (f).

References

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