1H-1T' heterocontact-induced polymorphism in monolayer CVD $MoTe_2$

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Molybdenum ditelluride ($MoTe_2$) has attracted increasing attention over the past few years, since it exists in two thermodynamically stable configurations, with peculiar electronic and structural properties. Monolayer (ML) 1H-$MoTe_2$ is a direct-gap semiconductor with an optical band gap of 1.10 eV [1], while 1T'-$MoTe_2$ is a semimetal and a 2D topological and large-gap quantum spin Hall (QSH) insulator [2]. Such properties make $MoTe_2$ an interesting material for applications in spintronics and quantum computing, as well as a perspective candidate for phase-change devices [3]. We report on high temperature polymorphism from single-crystal 1H to mono- or polycrystalline 1T', occurring at 730 ˚C in ML $MoTe_2$ grown by chemical vapor deposition (CVD), significantly lower temperature than the 1075 ˚C previously reported for exfoliated monolayer [4]. We present experimental AFM/KPFM/Raman/μXPEEM/XPS characterization of the hBN/Graphene encapsulated $MoTe_2$ samples. Experimental studies of ML samples are made possible by our newly developed encapsulation method [5]. We discuss strain effect and examine a new 1H-1T' heterocontact induced PT mechanism via DFT calculations. Our reported results open new perspectives in the $MoTe_2$ based micro- and nanoelectronics fabrication, phase-change devices and can be further studied in other TMDs, Janus materials [6]. This work has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement 881603. We acknowledge that the research activity herein was carried out using the IIT HPC infrastructure.

References

[1] Ruppert, C.; Aslan, O. B.; Heinz, T. F. Nano Lett. 2014, 14 (11), 6231−6236.
[2] Qian, X.; Liu, J.; Fu, L.; Li, J. Science 2014, 346 (6215), 1344−1347.
[3] Zhang, Feng, et al. Nature materials 18.1 (2019): 55-61.
[4] Ryu, Huije, et al. Advanced Functional Materials (2021): 2107376.
[5] Pace, Simona, et al. ACS nano 15.3 (2021): 4213-4225.
[6] Zhang, Lei, et al. Journal of Materials Chemistry A 8.18 (2020): 8813-8830.

Figures

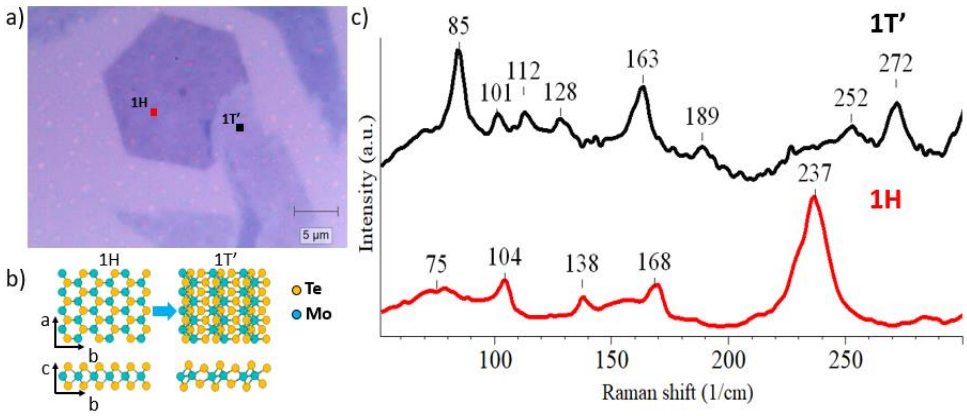

Figure 1: a), Optical image of the heterocontact-induced 1H to 1T' PT. b), Top and side views of 1H and 1T'-$MoTe_2$ ball-and-stick models. c), Raman spectra for the 1H and transformed 1T' regions in a).