Polymorphism in monolayer $MoTe_2$-based vertical VdW heterostacks

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Two dimensional (2D) molybdenum ditelluride ($MoTe_2$) is known to exist in two structural polymorphs: semiconductive (H) and semimetallic (T'), with extremely low ground state energy difference (30 meV/f.u.). H-$MoTe_2$ is a semiconductor with an optical band gap of 1 eV [1], while T'-$MoTe_2$ is a semimetal, which transforms into Weyl semimetal (Td) upon cooling [2]. Such properties make $MoTe_2$ an interesting material for phase-change devices. Achieving controllable and reversible phase transformation between these two phases shall impact the development of $MoTe_2$-based electronic devices. In this work, we show how by using mono- and few-layer T'-$MoTe_2$-based heterostructures encapsulated with CVD grown graphene, the T'/H to 2H energy barrier can be effectively controlled, which is appealing to devise approaches for energy barrier reduction and phase stabilization. Experimental studies are made possible by our newly developed encapsulation method [3]. We demonstrate that CVD bilayer 1T'/1H (1H/1T') either monolithic or synthetic can convert to 2H at about 600 °C, a lower temperature than the 800 °C required for $MoTe_2$ 1T'/1H phase transition when the material is encapsulated with CVD graphene. Also, we observe a 1T' to 1H-$MoTe_2$ phase transition at 750 °C in a vertical $MoTe_2$/WS_2/graphene VdW heterostructure. We propose an effective quantitative approach for estimating the experimental kinetic energy barrier between 1H/1T' and 2H phases, which agrees well with theoretical simulations. Furthermore, we report that upon annealing of 2H-$MoTe_2$ above 800 °C, we observe the formation of continuous Mo_6Te_6. This temperature is higher than the critical temperature of 400 °C reported for non-encapsulated $MoTe_2$ previously [4], and further suggests that adopting CVD grown graphene as an encapsulant can offer interesting prospects for phase control and phase-change device engineering. 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

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Figures

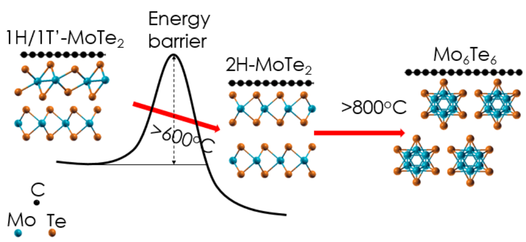

Figure 1: Schematics of the observed polymorphism