Vapor transport deposition of Transition Metal Tellurides (TMTs) and Ultra-Thin Tellurium nanosheets through Simulation-Guided Tellurization

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Tellurium-based two-dimensional (2D) materials possess unique characteristics that show potential as useful materials in various technological fields, spanning from nano-electronics to thermoelectric and energy sectors.[1] Specifically, 2D transition metal ditellurides (TMTs) can display either semiconductor or metallic properties based on their crystal phase structure, namely trigonal prismatic or octahedral. Among TMTs family, molybdenum ditelluride ($MoTe_2$) shows significant attention due to its polymorphic nature from semiconductor to topological insulator and Weyl-semimetal. [1-3] Similarly, the electronic and optical characteristics of 2D mono-elemental form of Tellurium (known as Tellurene) are greatly influenced by both its allotrope form and number of layers. In the α-phase, the most stable allotrope form in bulk, the electronic bandgap ranges from 0.92 eV in monolayer state to 0.33 eV in the bulk state.[4] To date, considerable efforts have been devoted for synthesizing large area $MoTe_2$ suitable for the fabrication of devices to be integrated in different applications. From this point of view, a precise synthesis of phase-selected, uniform $MoTe_2$ is essential.[2][3] Among many growth methods, chemical vapor deposition (CVD) is a facile and promising way for synthesizing large scale $MoTe_2$ nanosheets.

In this work, we thoroughly elaborate on the large scale and accurate phase-controlled growth of $MoTe_2$ films and atomically thin tellurium by CVD methods, demonstrated a correlation between the concentration gradient of Te vapor and the deposited $MoTe_2$ morphology and coverage.[2] We also developed a finite element simulation model (FEM) to understand the influence of experimental parameters, such as the substrate orientation, on the structural, morphological, and physical properties of the so-grown materials. Taking the advantage of FEM simulation guided experiments, we demonstrated a feasible CVD route for large scale growth with controlled phase tuning strategies for obtaining 1T'(metallic), 1T'/2H, and 2H (semiconducting) $MoTe_2$ nanosheets via tellurization of pre-deposited Mo thin film.[2] We show a detailed study of the heterogeneous vapor-solid reaction between a e-beam pre-deposited molybdenum film and tellurium vapor, thus yielding a large area growth of $MoTe_2$ onto SiO_2/Si substrate. Here, $MoTe_2$ growth and its phase selection is mainly influenced by the involved kinetics, tellurium concentration and geometry configurations inside the CVD furnace. Further, we expand our simulation guided tellurization methodology to realize other TMTs such as $PtTe_2$, $NiTe_2$. This study is a crucial step for enabling TMTs integration in numerous potential applications in novel micro- and nano-electronics to thermoelectric devices.

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