Ambient pressure chemical vapor deposition of Tellurium based 2D layers

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The peculiar properties of tellurium-based two-dimensional (2D) materials make them promising candidates for technological applications, ranging from nano-electronics to thermoelectric and energy fields [1,2,3]. Specifically, 2D transition metal ditellurides (TMTs) exhibit semiconducting or metallic behavior depending on the crystal phase structure: trigonal prismatic or octahedral. Moreover, in the semiconducting phase, they exhibit a transition from indirect to direct bandgap when thinned down from bulk to monolayer [4].

In analogy, 2D elemental form of tellurium (Tellurene) exhibits electronic and optical properties strongly dependent on the allotropic form, as well as on the number of layers. In the case of the α-phase, the most stable in the bulk form, the electronic bandgap varies from 0.92 eV in the monolayer state towards 0.33 eV in the bulk state [5]. For these reasons, the development of techniques capable to obtain controlled and large area 2D TMTs and tellurene layers is highly demanded. A reliable method is ambient pressure chemical vapor deposition (AP-CVD), which is flexible and may be adapted to the industrial production scale.

In this work, we report on large-area and uniform growths of atomically thin tellurium and MoTe2 films by AP-CVD methods [6,7]. We also develop finite element simulation models (FEM) to predict the effect of the experimental parameters, such as the substrate orientation, on the structural, morphological and physical properties of the so-grown materials. Exploiting the FEM simulations as a guide for the experiments, we show that there is a relation between Te vapor concentration gradient and the morphology and coverage of deposited $MoTe_2$. Notably, we also demonstrate that it is possible to finely control the allotropic phase of the grown few layers of $MoTe_2$ from the metallic 1T' phase to the 2H semiconducting phase, thus opening the way to a phase engineering of the material at the 2D limit [7]. Our findings are supported by atomic force microscopy (AFM) operating in different configuration, such as kelvin probe, conductive, tapping modes, as well as Raman and optical spectroscopies.

In extension, as a further outcome, we also show that the simulation-guided AP-CVD method can be easily extended for the growth of other tellurium based TMTs, such as $PtTe_2$, $NiTe_2$ and $AuTe_2$.

References (if needed)

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