THIRD YEAR PhD REPORT

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RESEARCH ACTIVITY

During the final year of my PhD project I mainly focused on the fabrication of van der Waals heterostructures based on 2D materials combining the know-how I acquired in the previous two years, i.e. the large area growth of few-layer Transition Metal Dichalcogenide (TMD) semiconducting films (MoS_2 and WS_2) recurring to an original physical deposition technique followed by a high temperature recrystallization process and large area transfer of commercial graphene on dielectric substrates.

Some results of the main activities of my research project are still missing due to the pandemic diseases, for which I received a three-months PhD extension.

- TMDs heterostructures self-powered devices

Due to the suitable bandgap range, few-layer TMD films and TMD vdW heterostructures are studied as promising materials for optoelectronics, photodetection and photoconversion. As an explorative experiment on the optoelectronic properties of our materials, I fabricated a large area WS_2/MoS_2 stack on top of a graphene electrode. Even if we measured very low I_{SC} and V_{OC} under broadband illumination conditions, we demonstrate the fabrication of a working self-powered device. The poor performance is attributed to the high resistance of the graphene on a macroscale and to possible shunts in the growth in the TMD layers. Nevertheless, the fabrication process can be further optimized to achieve better results.
A possible implementation that I am exploring is the addition of an Indium Tin Oxide (ITO) thick layer (about 50nm) beneath the graphene, that is expected to strongly reduce the resistance because of the vertical conduction through the graphene, instead than an in-plane conduction along several millimeters. The main challenge I am facing is the sulfurization on ITO, that even sulfurizing at a lower temperature reacts with sulfur losing its conductivity. A preliminary result achieved by capping ITO with graphene show promising conductivity, paving the way to an approach that could work even at higher temperature, enabling direct sulfurization of a WS_2/MoS_2 stack on top of ITO/graphene transparent electrode.

- TMDs for photocatalysis

In the last year a photocatalytic set-up haves been optimized in our laboratory. Specifically, we are working on the methylene blue (MB) photobleaching reaction as a test bench. The latter is a relevant reaction in the field of wastewater remediation being the MB a common dye molecule used by textile industries. TMDs are interesting materials for photocatalysis due to a favorable energy bandgap and to an extremely high surface to volume ratio, so we decided to explore these materials as an alternative to the previously explored plasmonic approach (based on gold nanowires).
In this context, I worked on the fabrication of TMDs ultrathin films for MB photobleaching. Both MoS_2 and WS_2 samples showed enhanced photobleaching with respect to the gold nanowires. Additionally, vertically stacked van der Waals (vdW) heterostructures between MoS_2 and WS_2 represent a promising solution as they form a type II heterojunctions, in which photogenerated electron-hole pairs can be physically separated in the two different layers resulting in a longer lifetime for the free carriers on the surface involved in the MB photobleaching. Preliminary experiments indeed show an increased reactivity in the case of a WS_2/MoS_2 stack.

- MoS_2 engineering with low energy Ar plasma

To improve the electric properties of our MoS_2 films I am trying to induce a transition from the semiconducting 2H phase to the metallic 1T phase by sputtering with a low energy argon plasma. Preliminary results are currently under examination. In an interesting development to be performed in the last months of my thesis, I plan to explore a nitrogen plasma to induce doping in the 2D material.

- Grating morphology modification via Ion Beam Sputtering

The possibility to modify the morphology of the templates on which 2D materials are grown can pave the way to powerful optical engineering. For this purpose, I devoted effort at tailoring the faceted morphology by sputtering the nanogrooved silica templates at different off-normal angles in order to control the slope of the ridges. The templates are optimized for an experiment aiming at color routing via Mie scattering using high refractive index TMD materials. Morphology tailoring results are currently under examination.

PUBLICATIONS

- M.C. Giordano, G. Zambito, M. Gardella, F. Buatier de Mongeot, "Thermal sculpting of 2D-TMD semiconducting nanocircuits at wafer scale", under review
- G.Ferrando, M. Gardella, G. Zambito, M. Barelli, D. Chowdhury, M.C. Giordano, F. Buatier de Mongeot, "Flat optics Hybrid MoS_2/polymer films for photochemical conversion", submitted

CONFERENCE PRESENTATIONS

- European Materials Research Society 2022 Spring Meeting, online
    - Oral contribution: 'Large-area 2D-TMDs heterostructures engineered for enhanced light harvesting'
    - Oral contribution: 'Optical anomalies in large-area MoS_2 nanoripples boost photobleaching of dye molecules'
- 22nd International Conference on Ion Beam Modification of Materials 2022, Lisbon
    - Oral contribution: 'Tailoring Of Two-Dimensional Semiconductors Optoelectronic Properties Via Ion Induced Nanopatterning'
    - Poster contribution: 'Maskless Ion Beam Sputtering Deposition Of Two-Dimensional Transition Metal Dichalcogenides Van Der Waals Heterostructures'
- Micro and Nano Engineering Conference 2022, Leuven
    - Poster contribution: 'Deterministic growth of semiconducting MoS_2 nano-patterns via thermal – Scanning Probe Lithography (t-SPL)'