1L-MoS2 on SiO2 Photoluminescence Enhancement Via Post-Synthesis Thermal Treatments

Antonino Madonia*[1], Emanuele Sangiorgi[1], Francesca Migliore[1], Gianmarco Laurella[1], Salvatore Ethan Panasci[2], Emanuela Schilirò[2], Filippo Giannazzo[2], Fiorenza Esposito[3,4], Luca Seravalli[3], Igor Píš[5], Federica Bondino[5], Gianpiero Buscarino[1,6], Marco Cannas[1], and Simonpietro Agnello[1,2,6]

[1]Department of Physics and Chemistry, University of Palermo (UNIPA) – Via Archirafi 36, 90143 Palermo (Italy), Italy

[2]Consiglio Nazionale delle Ricerche, Istituto per la Microelettronica e Microsistemi (CNR-IMM) – Strada VIII, 5, Zona Industriale, I-95121 Catania (Italy), Italy

[3]Consiglio Nazionale delle Ricerche, Istituto dei Materiali per l'Elettronica ed il Magnetismo (CNR-IMEM) – Parco Area delle Scienze 37/a, 43124 Parma (Italy), Italy

[4]University of Parma, Department of Chemical Science, Life, and Environmental Sustainability – Parco Area delle Scienze 7/a, 43124 Parma (Italy), Italy

[5]Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali (CNR-IOM) – Area Science Park, S.S. 14 Km. 163, 5, Basovizza, I-34149 Trieste (Italy), Italy

[6]ATEN Center, University of Palermo (ATEN) – Viale delle Scienze Ed. 18, 90128 Palermo (Italy), Italy

Abstract

Abstract

The impact of post-synthesis thermal treatments under controlled atmospheres on the optical properties of monolayer molybdenum disulfide (1L-MoS2) on SiO2 was explored. This research highlights how the synthesis affects the material's photoemission characteristics, closely linked to strain and doping levels. By employing thermal treatments, predictable changes in strain and doping were observed. Comparisons of flakes from different production methods revealed improvements in optical performance post-treatment, suggesting a viable approach to address the shortcomings of production techniques. These findings underscore the potential of tailored post-synthesis processes to enhance the optical properties of 2D materials, crucial for advanced optoelectronics applications. The research aims to optimize photonic devices based on MoS2 and other transition metal dichalcogenides, emphasizing the significance of controlling structural and electronic characteristics in achieving the desired material's properties.

Introduction

Recent advancements in two-dimensional (2D) materials have opened new avenues for industrial applications, particularly in optoelectronics.(1) Among these, heterostructures made of stacked 2D layers with complementary features have garnered significant attention due to their unique properties. Monolayer Van der Waals materials, such as semiconducting transition metal dichalcogenides (TMDs), are especially valuable because of their atomic-scale

*Speaker

thickness, direct bandgap, and excellent electronic and mechanical properties.(2)

Monolayer molybdenum disulfide (1L-MoS2) stands out as a model material within this family. It has been extensively studied due to its intense photoemission at 1.8eV, which originates from direct excitonic recombination.(3) This property is closely linked to the material's strain and doping levels. However, defects introduced during synthesis can significantly impact its optical performance.(4)

Our research focuses on understanding how post-synthesis thermal treatments under controlled atmospheres influence the properties of 1L-MoS2.(5) We observed predictable changes in strain, doping, and emission characteristics of the material after these treatments. By comparing flakes obtained through different preparation methods, we found that the optical properties improved after treatment, suggesting a way to mitigate the drawbacks of certain production techniques.

Materials and methods

Monolayer molybdenum disulfide (1L-MoS2) flakes were synthesized by gold-assisted exfoliation or chemical vapor deposition (CVD). The flakes were transferred onto insulating SiO2 substrates, and a comparison was carried out employing either conductive Au or semiconducting GaN substrates. The samples were then subjected to thermal treatments in a Linkam thermal cell at temperatures ranging from 100◦C to 300◦C under 2bar O2 or Ar atmospheres for durations between 30 minutes and 20 hours. Characterization was performed by Raman spectroscopy, which allowed to analyze the strain and doping conditions, as well as the effects of thermal treatments. Additionally, the optical properties of the material were studied via micro-photoluminescence while atomic force microscopy was used to examine the flake structure and morphology. Finally, synchrotron-radiation X-ray photoelectron spectroscopy (XPS) was performed to elucidate changes in the chemical composition.

Main Results

From the position of the E' and A' Raman bands it is possible to study the strain and doping of 1L-MoS2.(6) As demonstrated in Figure 1, thermal treatments under an O2 atmosphere can reduce the negative-charge carrier concentration in flakes grown by CVD on SiO2 substrates. This result was studied in detail for different treatments temperatures and durations. Additionally, comparing results obtained under O2 and Ar atmospheres suggests that oxygen is able to fill the sulfur vacancies inherent to the material structure. Such consideration was further supported by the results of XPS measurements.

Figure 1: Strain-doping map of 1L-MoS2 grown on SiO2 by CVD before and after 2 hours-long thermal treatments carried out under 2 bar of O2 at different temperatures.

Furthermore, each treatment lead to a significant increase in the 1L-MoS2 photoluminescence intensity, as shown in Figure 2. Such effect was not observed for treatments carried out in Ar, highlighting the fundamental role of O2 in the witnessed effects.

Figure 2: Photoluminescence of 1L-MoS2 grown on SiO2 by CVD before and after 2 hours-long thermal treatments carried out under 2 bar of O2 at different temperatures.

These findings, proven viable regardless of the preparation method used to obtain the flakes, pave the way for further research into optimizing optical devices based on 1L-MoS2 and other TMDs and demonstrate the potential of tailored post-synthesis treatments to enhance the optical properties of 1L-MoS2. An in-depth comparison with other substrates will be presented to elucidate the role of SiO2.

Acknowledgements

This research was funded by the Italian MUR PNRR project SAMOTHRACE (ECS00000022) and the PRIN 2022 project titled 2D materials Integration with Nitride semiconductors for advanced Electronics (2DIntegratE) (2022RHRZN2) under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union-NextGenerationEU.

References

(1) Lemme, M.C., et al. Nat. Commun. 13, 1392, 2022.

(2) Geim, A.K. et al., Nature 499, 419–425, 2013.

(3) Mak, K. F., et al., Phys. Rev. Lett. 105, 136805, 2010.

(4) Zhou, W. et al., Nano Lett. 13, 2615–2622, 2013.

(5) Sangiorgi, E. et al., Nanomaterials 15, 160, 2025.
(6) Michail, A., et al., Appl. Phys. Lett. 108, 173102, 2016.

Keywords: MoS2, 2D materials, thermal processing, strain, doping