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Thermal-Induced Defects in Monolayer MoS_2 Flakes

U. Defect-induced effects in low-dimensional and novel materials

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Abstract

Transition metal dichalcogenides are semiconducting materials of high appeal for their significant charge carrier mobility and intense optical properties.[1] Molybdenum disulphide in particular presents a thickness-dependant band-gap which gives rise to direct transitions between its valence and conduction band when reduced down to monolayers. Such effect along with its high absorption coefficient allows for an intense photoemission.[2] Thanks to its large natural abundance when in bulk form and to the simple approaches that allow to exfoliate and transfer its flakes to other substrates, MoS_2 has often been used for the development of a wide range of optoelectronic devices such as transistors, photodetectors and light emitting diodes.[3] However, MoS_2 properties are strongly altered by the doping and strain condition of the monolayer.[4] Additionally, the remarkable tendency of such material to interact with the environment and surrounding molecules allows for aging processes ultimately causing defects and thus affecting the final properties of the monolayer flakes.[5] In order to better understand the causes of such aging we have carried out thermal treatments on MoS_2 under controlled atmosphere of Ar, N_2, O_2 and air between 150°C and 300°C. By following individual monolayers through techniques such as atomic force microscopy, Raman and photoluminescence spectroscopy we were able to explore this material stability and the reversibility of the defect-inducing processes. Overall we were able to find that changes in the stress and doping of the material can be effectively tuned by the thermal treatments, although affected by the different atmospheres. In particular, we have observed how the MoS_2 crystalline structure stress caused by the production methods and the subsequent transfer to a substrate can be reduced during the thermal treatments. Moreover, the characteristic photoemission bands due to exciton recombination are affected in peak position and intensity depending on both treatment duration and gas in the atmosphere. Our approach demonstrates that the alterations in the material's properties are permanently retained after going back to room temperature, thus

allowing to control and reduce the effects of the aging processes.

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