Defect activated Raman modes and bound-excitons correlation in monolayer WS_2

L. M. V. Ildefonso[a], **E. L. Buthers**[b], **W. R. Ramos**[a], **A. N. F. Diniz**[a], **R. L. Falcão**[a], **J. S. Souza**[a], **Y. C. Santos**[a], **C. Legnani**[a], **W. G. Quirino**[a], **D. V. P. Massote**[a], **B. S. Archanjo**[b], **I. O. Maciel**[a] e **B. Fragneaud**[a]

a) Universidade Federal de Juiz de Fora, Departamento de Física

b) Instituto Nacional de Metrologia, Qualidade e Tecnologia, Divisão de Materiais

Resumo

In recent years, transition metal dichalcogenides (TMDs) have been widely studied due to their unusual optoelectronic properties. Recently, the study of defects in these materials allows the application in semiconductor devices, since defect sites locally disturb the crystalline lattice, leading to peculiar effects. For example, punctual defects (zero-dimensional) are the single-photon emission source, which is an important role in the quantum information devices industry [1], and highly ordered defect lines (one-dimensional) exhibit charge wave densities along themselves [2]. In this context, Raman and photoluminescence spectroscopies have been a powerful tool to quantify and identify structural defects in 2D materials. In this work, we synthesized monolayers of WS_2 via chemical vapor deposition (CVD), bombarded these samples with He ions and we verified the existence of two Raman bands and two new electronic transitions, present in the photoluminescence spectra, activated by punctual defects. First-principle calculations were performed to obtain the electronic and phononic dispersion, thus inferring the origin of the observed effects in Raman and PL spectra. The same punctual defect model that allows to predict the crystallinity of graphene and molybdenum TMD [3] was employed to visualize when WS2 begins to become amorphous. From these analyses, it was possible to build the correlation between Raman-active modes due to defects and bound excitons. So, this work makes possible the identification of defects in tungsten TMDs, which are much used in the technology industry of semiconductors.

REFERENCES

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e-mail: leticia.ildefonso@estudante.ufjf.br