Raman spectroscopy in black phosphorus edges

Henrique B. Ribeiro[1]
C. E. P. Villegas[3], D. A. Bahamon[1], D. Muraca[4], A. H. Castro Neto[5], E. A. T. de Souza[1], A. R. Rocha[3], M. A. Pimenta[6] and C. J. S. de Matos[1]

[1]*MackGraphe—Graphene and Nanomaterials Research Center, Mackenzie Presbyterian University, 01302-907 São Paulo, Brazil.*
[2]*Istituto di Struttura della Materia of the National Research Council, Via Salaria Km 29.3,I-00016 Monterotondo Stazione, Italy*
[3]*Instituto de Física Teórica, Universidade Estadual Paulista Julio de Mesquita Filho (UNESP), 01140-070 São Paulo, Brazil.*
[4]*Instituto de Física Gleb Wataghin (IFGW), Universidade Estadual de Campinas, 13083-970 Campinas, Brazil.*
[5]*Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore 117546, Singapore.*
[6]*Departamento de Física, Universidade Federal de Minas Gerais (UFMG), 30161-970 Belo Horizonte, Brazil.*

henfisica@gmail.com

Abstract

Black phosphorus (BP) is a thermodynamically stable allotrope of phosphorus, possessing a lamellar structure, which allows the production of its crystal in the two dimensional form [1]. Its band structure is dependent of the number of layers, with which its band gap varies from 0.3eV to 2.0eV [2], making it ideal for fabrication of optic and optoelectronic devices. Also, its puckered structure confers anisotropic properties that are optically manifested, on the optical absorption and Raman scattering. In this work, a black phosphorus crystal was exfoliated into a silicon substrate with a 300nm thickness of silicon oxide top layer and hyperspectral imaging were performed in flakes with well-defined crystallographic edges. The Raman images were obtained in two configurations, where the polarized incident light was either parallel or perpendicular to an analyzer, placed before the spectrometer.

From the Raman measurements, we observe the appearance of modes, at the edges, that should not be present in the measured polarization configuration. In order to explain these new features, density functional theory (DFT) simulations were performed, in which the experimental results were reproduced. From the experimental data and DFT simulations we conclude that the observed Raman features arise due to atomic rearrangements at the edges [3], a feature that is not observed in graphene, for example.

References

[1] A. Castellanos-Gomez, Leonardo Vicarelli, Elsa Prada, Joshua O Island, K L Narasimha-Acharya, Sofya I Blanter, Dirk J Groenendijk, Michele Buscema, Gary A Steele, J V Alvarez , 2D Mater. Journal, 1(2) (2014) 025001

[2] Tony Low, A. S. Rodin, A. Carvalho, Yongjin Jiang, Han Wang, Fengnian Xia, and A. H. Castro Neto, Phys. Rev. B., 90, (2014), 075434

[3] H. B. Ribeiro, C. E. P. Villegas, D. A. Bahamon, D. Muraca, A. H. Castro Neto, E. A. T. de Souza, A. R. Rocha, M. A. Pimenta and C. J. S. de Matos. Nat. Commun., 7, (2016), 12191.

Acknowlegements

This work is supported by FAPESP (SPEC project 2012/50259-8 and Thematic project 2015/11779-4), INCT/Nanocarbono, Fapemig, CNPq and MackPesquisa.