黄昆半导体科学技术论坛

 **第327期讲座**

**报告题目:Double-Resonant Raman Processes in Single Layer Graphene, Carbon Nanotubes and Twisted Bilayer Graphene**

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**Abstract**: Lowest-order Raman processes, for instance the G band in graphene, correspond to the scattering with a zero-momentum phonon (**q = 0**). Graphene and graphitic materials present other lines, due to higher-order processes, which are usually interpreted in terms of the so-called double-resonance (DR) mechanism. The DR mechanism is used to interpret RamanD band and 2D band in graphene. We have developed a methodology, based on Density Functional theory, to simulate the DR processes in graphene[1].

Here we show that the Raman bands related to DR processes are a powerful tool to probe the structural, electronic and vibrational properties of graphitic materials. We will focus in three different systems: monolayer graphene, carbon nanotubes and twisted bilayer graphene.In monolayer graphene, the observed 2D line width contains valuable information on strain variations in graphene on length scales far below the laser spot size, that is, on the nanometer-scale[2], which is a good and easily accessible quantity for classifying the crystalline quality, nanometer-scale flatness as well as local electronic properties of graphene.Concerning carbon nanotubes, we have studied the D and 2D Raman bands of chirality enriched samples[3]. We show that each single-chirality nanotube exhibits a series of non-dispersive D and 2D Raman peaks, which are not necessarily enhanced by resonances with optical transitions between van Hove singularities. Our results provide a complete explanation of the DR Raman spectrum, including the D and 2D bands, at the specificity level of a single-chirality nanotube, and allow the correct interpretation of the DR spectra of carbon nanotubes in samples containing a distribution of different (n, m) nanotube species.Finally, for twisted bilayer graphene[4], we discuss the possibility of distinguishing intralayer and interlayer electron-phonon (el-ph) interactions and of probing the intralayer process in graphene/h-BN. In the intralayer process, the el-ph scattering occurs in a single graphene layer and the other layer (graphene or h-BN) imposes a periodic potential that back scatters the excited electron, whereas for the interlayer process the el-ph scattering occurs between states in the Dirac cones of adjacent graphene layers. Our methodology of using Raman spectroscopy to probe different types of el-ph interactions can be extended to study any kind of graphene-based heterostructure.

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**Acknowledgments:**PV acknowledges the support of the brazilian agencies: CNPq, Capes and Faperj.

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**Biography:** PV earned his PhD at Universidade de São Paulo in Brazil in 1996. After that he was a pos-doc at IBM research center in Yorktown Heights, USA. Since 2002 he is a faculty at Universidade Federal Fluminense, in Niterói, Rio de Janeiro, Brazil. He has worked with electronic structure of materials and recently specially with 2D materials. In 2009/2010 he spent a sabatical year at Université Pierre at Marie Curie in Paris, where he started studying Raman spectroscopy in 2D materials in a theoretical point of view.

**时间: 2018年9月3日(星期一) 下午3：30**

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