Full 2D calculation of graphene Raman amplitude

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Graphene Raman spectra make it possible to deduce about amount of monolayers and their distribution in the sample and the defect structure of the sample. Here we make a calculation of graphene Raman spectra. The calculation for graphene bilayer is provided. Also we consider the substrate effect for graphene monolayer.

The calculation of graphene Raman spectra requires its electronic structure and phonon dispersion [1]. We use the harmonic approximation [2] to obtain the phonon dispersion of graphene. Interatomic force constants utilized in this work were taken from [3]. Accurate approximation of the experimentally obtained phonon dispersion in spite of phonon dispersion full calculation can be also implemented. On the contrary, the utilization of interatomic force constants opens up possibilities of the substrate and number of layers effects consideration.

Raman spectra are calculated on the basis of the amplitude of double resonant processes. Defect-induced processes corresponds to the D band and corrections for the G band. Processes which involve two phonons corresponds to overtones: 2D and 2G bands.

We provide the calculation for the bilayer graphene. In the bilayer graphene electronic bands splits [4] and four types of electron transitions appears. It results in the fact that 2D gets more broad. This broadening agrees with experimental data.

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