

Phonon dispersion and Raman spectra of graphene and graphene layers on gold substrate

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The phonon dispersion of graphene displays two strong Kohn anomalies in the highest optical branch at the high-symmetry points Γ and K [1]. This phenomenon is related to the electron-phonon coupling with the graphene π bands and has a strong influence on Raman scattering. The interaction between graphene and metallic substrate can significantly modify the electron-phonon coupling thus the Raman spectra can be used to identify the type of doping together with determination of number of graphene layers and their electronic structure [2, 3]. In this work, we analyze the influence of gold substrate on the phonon dispersion of the graphene and graphene multilayer calculated with DFT-LDA and Van der Waals density functional. The simultaneous analyzes of the Raman spectra, e.g. the changes in shapes, widths and positions of D, G and 2D peaks, allows to identify first of all the number of graphene layers, next substrate influence on their electronic properties as well as the nature of doping and its probable source.

In Fig.1 we present the schematic view of the sample used in the Raman experiment. Measured Raman spectra with laser line 514 nm for different places of the sample are shown in Fig. 2. The layer number of graphene has been identified by analyzing the shape of 2D band. We could indicate 4 regions: monolayer, bilayer, trilayer and few layers. The simultaneous up-shifts of the G and 2D band positions confirm [4] the p-doping in the graphene/Au system. The accurate DFT calculations analyzed together with the computed phonon frequencies lead to the determination of the electron-phonon coupling which allows to understand and explain the observed p-doping.

This work was financially supported by Polish Ministry of Science and Higher Education in the frame of grant N N202 204737.

References

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Figures

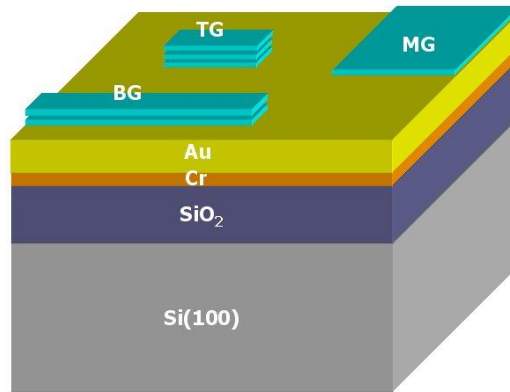


Fig. 1

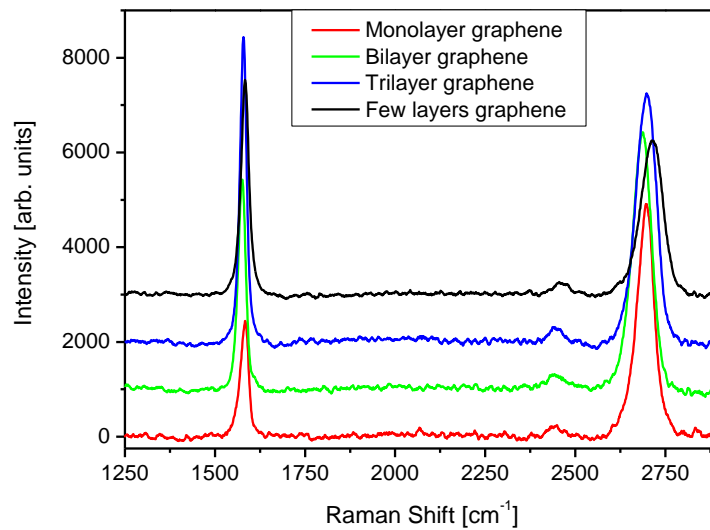


Fig. 2

Fig. 1 Schematic view of a sample

Fig. 2 Raman spectra of mono-, bi-, tri-, and few layers graphene deposited on Au substrate.