Interface Effect on Dielectric Function of Graphene from Ellipsometry and First-Principles Study

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With its extraordinary optical properties and thermal conductivity, the two-dimensional carbon allotrope graphene has demonstrated as an excellent candidate in solar cells, microelectronics, optoelectronics, etc. Recently, graphene has been massively produced and deposited on various substrates by the Chemical Vapor Deposition (CVD) method. Yet the different choices of substrate greatly influence the optical properties of deposited graphene. Thus, to broaden and deepen its wide application in the scientific community, it's crucial to understand and predict the interface effect on the thermophysical parameter dielectric function of graphene deposited on different substrates. In this work, the dielectric functions of graphene deposited on metal copper and quartz crystal are wholly investigated by the ellipsometry experiments and first-principles calculations. The state-of-the-art infrared-variable angle spectroscopic ellipsometry (IR-VASE) and visible-variable angle spectroscopic ellipsometry (V-VASE) are applied to experimentally measure the room-temperature dielectric functions of graphene spanning from the spectral range 0.19-33 μm. By comparing the measured dielectric functions of graphene deposited on the two different substrates with that of isolated graphene from previous literatures, the interface effect is analyzed and discussed. On the other hand, to intrinsically understand and predict the interface effect, the first-principles methods are applied to calculate the electronic band structure and dielectric functions of isolated graphene and those deposited on metal copper and quartz crystal. The calculated dielectric functions of isolated graphene are compared with experimental measurements to verify the first-principles calculations. The electronic band structure and density of states of isolated and deposited graphene are investigated to intrinsically analyze and understand the interface effect. In sum, this works aims to provide some insight into understanding and predicting the dielectric functions of graphene deposited on different substrates.