SSF-O1

Microscopic description of a film of the single-walled carbon nanotube in the optical range

Mikhail Shuba[1], Gintaras Valušis[1] and Vasil Saroka[2]

[1] Optoelectronics Department, Center for Physical Sciences and Technology, Sauletekio av. 3, Vilnius LT-10257, Lithuania.

[2] Department of Physics, University of Rome Tor Vergata and INFN, Via della Ricerca Scientifica 1, 00133 Roma, Italy.

Email: mikhail.shuba@ftmc.lt

Films of single-walled carbon nanotubes (SWNTs) are promising for usage as transparent electrodes. Their optical response can be controlled through electrostatic doping. Despite the large amount of experimental data on the optical parameters of SWNT films, there is no theoretical approach for their satisfactory description. Currently, the quantum model of π-electron transitions is considered to be the most appropriate to describes the optical resonances in SWNTs associated with interband electron transitions [1]. However, this model cannot adequately describe the contribution to the optical response caused by the UV π-plasmon in SWNTs.

In this work, we propose to include in the existing quantum mechanical model of SWNT conductivity additional terms that take into account phenomenologically the ultraviolet pi-plasmon, as well as the contribution from σ-electrons [2]. The parameters of additional terms are proposed to be determined from experimental data obtained for the optical conductivity of graphene. Such a microscopic approach makes it possible to describe the optical spectra of SWNT films. It predicts strong suppression of the transvers response of SWNTs due to the depolarization effect. In addition, the proposed approach satisfactorily describes the experiments [3] on observing an azimuthal plasmon in doped SWNT films. It explains why an azimuthal plasmon occurs for electrostatically doped SWNT films in ionic liquids and only for heavily doped SWNT films in the air.

We have also developed the scattering theory for SWNT bundle when the incident light is polarized perpendicular to the bundle axis. We showed that bundling cannot significantly change the height and frequency of the azimuthal plasmon peak in the absorption spectrum of the doped SWNT film.

The developed microscopic approach can be useful for the description of the optical parameters of SWNT films for different optoelectronic applications.

REFERENCES

[1] S. Tasaki, K. Maekawa, and T. Yamabe; *Phys. Rev. B* **57** (1998) pp. 9301-9318.

[2] M.V. Shuba, G. Valušis, V.A. Saroka; *Phys. Rev. B* **109** (2024) pp. 165409.

[3] D. Satco, D.S. Kopylova, F.S. Fedorov, T. Kallio, R. Saito, and A.G. Nasibulin; *ACS Appl. Electron. Mater*. **2** (2020) pp. 195-203.