Fresnel coefficients of a two-dimensional atomic crystal

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In general ellipsometry is able to furnish both the susceptibility and the conductivity of a bulk material. Here I will show how ellipsometry is able to furnish both the surface susceptibility χ and the surface conductivity σ of graphene. I fit the most remarkable experiments in graphene optics and I obtain, in the spectral range 450 nm < λ < 750 nm, a $\chi = 8\cdot10^{-10}$ m $\pm$ $3\cdot10^{-10}$ m and a $\sigma = 6.08\cdot10^{-5}\ \Omega^{-1} \pm 2\cdot10^{-5}\ \Omega^{-1}$[1]. While the value of σ has been reported several times [2], as far as I know, this is the first reliable determination of χ.

The experiments on the linear optical properties of a single-layer two-dimensional atomic crystal are usually interpreted by modeling it as a homogeneous slab with an effective thickness. Here the fit is done by using the Fresnel coefficients. It is shown that the Fresnel-based model and the slab-based model are not equivalent. This analysis indicates that the Fresnel-based model is able to simulate the overall experiments here analyzed, while the slab-based model fails to predict almost everything, and in particular the absorption and the phase of the reflected light.

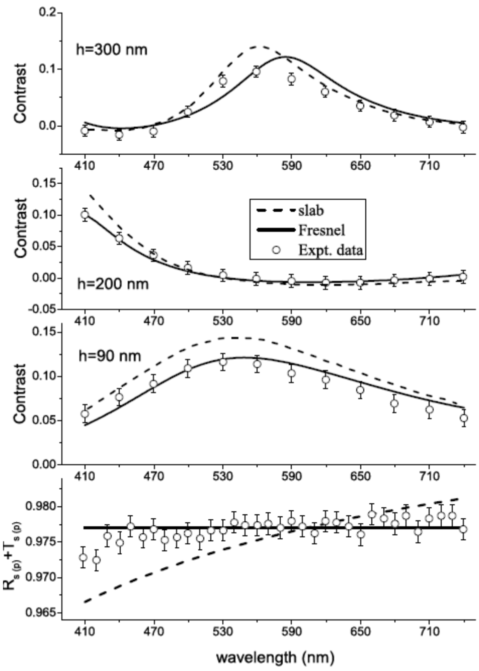

FIG. 1 The first three graphs show the optical contrast of graphene on SiO2/Si. The experimental data and the simulations based on the slab model are extracted from [3]. The last graph shows the absorption of a free-standing graphene layer. Experimental data are extracted from [2].

The experimental measurements here considered are absorption [2], optical contrast [3] and ellipsometry [4]. Figure 1 compares the experimental data and the slab-based model predictions published in [3] with the Fresnel-based model. The first three graphs give the optical contrast for single-layer graphene on top of SiO_2/Si wafers with three different SiO_2 thicknesses. Polarizations *s* and *p* give the same results. The Fresnel fit reported in the first three graphs of Fig. 1 is for $\sigma = 6.08\cdot10^{-5}\ \Omega^{-1}$ for and for $\chi = 5\cdot10^{-10}$ m. The last graph of Fig. 1 considers a free standing graphene layer and considers absorption. For a $\sigma = 6.08\cdot10^{-5}\ \Omega^{-1}$ the Fresnel theory predicts a constant absorption as a function of the wavelength whereas the slab model predicts a wavelength dependence. The two theoretical predictions are compared with the experimental data published in [2]. Already from Fig. 1 the superiority of the Fresnel-based model is quite evident. Anyway the optical contrast and absorption measurements are not able to discriminate very well the value of χ. All the Fresnel fits with $\chi < 10^{-9}$ m give in practice the same result.

To fix χ, I turned my attention to spectroscopic ellipsometry of graphene flakes located on a flat amorphous quartz. Figure 2 compare the theoretical predictions for the Fresnel-based model and for the slab-based model with the measurements published in [4]. It shows the simulated spectral dependence of the ellipsometric parameter Δ at four angles of incidence. A good Fresnel fit is obtained for $\sigma = 6.08 \cdot 10^{-5}\ \Omega^{-1}$ and for $\chi = 1.0 \cdot 10^{-9}$ m. This is compared with the slab-based model used in [4] in the same frequency range. At 55° Δ does not fit very well, maybe because of cross polarization effects. From Fig. 2 the Fresnel-based model fits much better than the slab-based model the experimental data for the ellipsometric parameter Δ, and hence it better predicts the phase of the reflected light. The ellipsometric parameter Δ is very sensitive to the graphene film because Δ= 180° or 0° for the quartz substrate and all the non trivial phase contribution to the reflection coefficients comes from graphene. In particular the phase of the reflected light is different from 180° or 0° only if $\chi \neq 0$ m. The experimental data for Δ allow to fix χ with a precision of $1 \cdot 10^{-10}$ m or better, and they are also sensitive to its sign. The Fresnel fit and the slab fit, for the ellipsometric parameter Ψ, are almost equivalent.

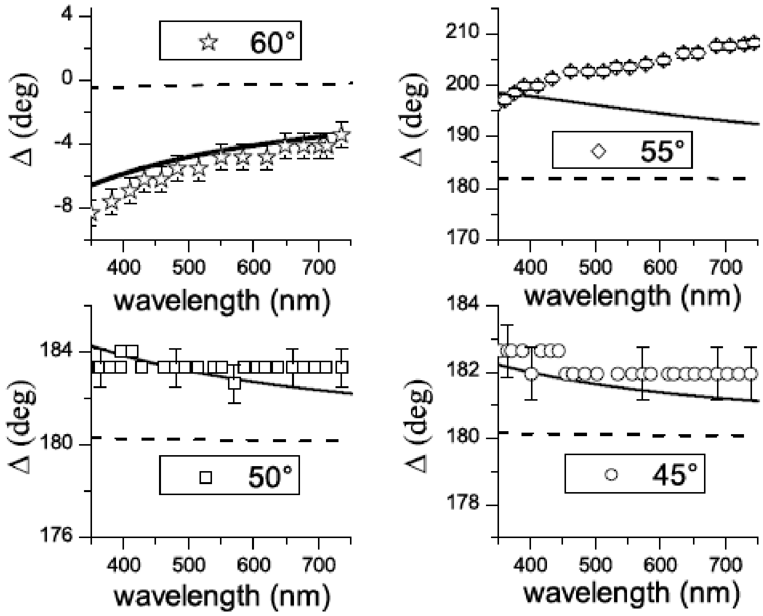

FIG. 2 Spectral dependence of the ellipsometric parameter Δ for graphene on an amorphous quartz substrate for each of the four angle of incidence considered in [4]. Experimental data are represented by dots, slab-model predictions by a dashed line and Fresnel-model predictions by a solid line.

In conclusion the comparison [1] with the experimental results shows that the Fresnel coefficients are essential to interpret the most remarkable experiments in graphene optics [2-4], fixing both σ and χ. Any hypothesis on an effective thickness of a single-layer 2D atomic crystal as required by modeling it as a homogeneous slab is not necessary. This last model is not able to reproduce properly either the absorption of graphene or the phase of its reflection coefficient. On this basis any physical parameter, deduced from it, is hardly meaningful.

References

[1] M. Merano, Phys. Rev. A **93** (2016) 013832.

[2] R. R. Nair, P. Blake, A. N. Grigorenko, K. S. Novoselov, T. J. Booth, T. Stauber, N. M. R. Peres, and A. K. Geim, Science **320** (2008) 1308.

[3] P. Blake, E. W. Hill, A. H. Castro Neto, K. S. Novoselov, D. Jiang, R. Yang, T. J. Booth, and A. K. Geim, Appl. Phys. Lett. **91** (2007) 063124.

[4] V. G. Kravets, A. N. Grigorenko, R. R. Nair, P. Blake, S. Anissimova, K. S. Novoselov, and A. K. Geim, Phys. Rev. B **81**, (2010) 155413.