# Anisotropic Permittivities and Transmittance of Double Layer Graphene

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## 1. Introduction

Graphene is a two dimensional material consisted of honeycomb carbon lattices. Comparing to pure graphene, bi-layer graphene is taking special interest due to the interlayer interactions. The interlayer coupling has the influences on the electronic and optical properties, which has crucial characteristics distinct from graphite. Ebernil *et al*. [1] reported that the single layer graphene has red-shifted surface plasmon modes from graphite at 4.7 eV and 14.6 eV. It illustrated that the dielectric function of graphene distinct from graphite. In this work, the permittivities of double layer graphene are numerically simulated using Density Functional Theory (DFT) method. Also, the transmittance of $SiO_2$ substrate model, surface conductivity approach of graphene model, and DFT model are compared.

## 2. Results and Discussions

The exchange-correlation function of simulations using Vienna Ab-initio Simulation Package [2] (VASP), which is based on the Kohn-Sham equation, are adopted for local density approximation. In this work, the dielectric function is determined through the summation of empty states [3].

The real and imaginary part of permittivities on double layer graphene are shown in Fig. 1. It should be noticed that only interband transition is considered in the calculation. The in-plane permittivity of imaginary part shows that the two peaks at 4 and 14 eV are due to $\pi$-$\pi^*$ and $\sigma$-$\sigma^*$ interband transitions, respectively. However, the peaks at 11 and 14 eV for out-of-plane polarization are due to $\pi$-$\sigma^*$ and $\sigma$-$\pi^*$ interband transitions. Near the zero energy, it illustrates semiconductor property for out-of-plane polarization and metallic property for in-plane polarization.

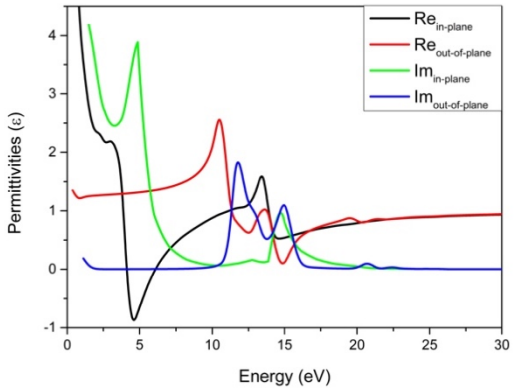


Fig. 1. Real and imaginary parts of permittivities of double layer graphene. Notice that only interband transition is considered in these cases.

As shown in Fig. 2, the transmittances of $SiO_2$ substrates model, surface conductivity approach of graphene model [4], and DFT model are compared using Finite Difference Time Domain (FDTD) methods. The wavelengths of incident light, which is in-plane polarization, are from 30 nm to 600 nm. The result of surface conductivity approach model is only adopted intraband transition, which is often applied in mid-infrared regions. However, the peak of DFT model near 300 nm located in ultraviolet region distinct from the surface conductivity model. Because the interband transition of surface conductivity model is ignored, the optical properties should be reconsidered in visible and ultraviolet regions. It is corresponded to fast changes of real and imaginary parts of in-plane polarization around 4 eV as shown in Fig. 1.

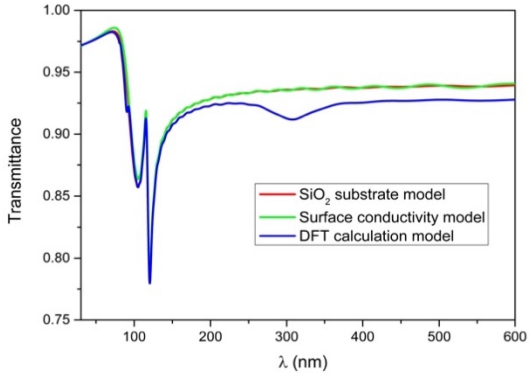


Fig. 2. The transmittances for three models.

## 3. Conclusions

The permittivities are strongly depended on polarizations. Near zero energy, the imaginary part of dielectric function exhibits metallic behavior for in-plane polarization and semiconductor behavior for out-of-plane polarization, respectively. Also, the transmittance difference between surface conductivity approach model and DFT calculation model shows importance of interband contribution in short-wavelength regions.

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## References

[1] T. Eberlein *et al*., Phys. Rev. B, **77** (2008) 233406.
[2] G. Kresse and J. Furthmüller, Phys. Rev. B **54** (1996) 11169.
[3] M. Gajdoš *et al*, Phy. Rev. B **73** (2006) 045112.
[4] L. A. Falkovsky, J. Phys.: Conf. Ser. **129** (2008) 012004.