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Understanding the microscopic origin of Terahertz conductance in strained polycrystalline graphene

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The conductivity of polycrystalline graphene in the THz range is relevant for many applications. However, a full understanding of the underlying physics has not yet been achieved, due to the lack of reliable models of carrier transport in polycrystalline nanomaterials. In this work, we relate the structural deformation in strained graphene with the deviation from the Drude conductance. To this end, THz time-domain spectroscopy has been performed as function of the graphene deformation to extract the frequency dependence of the permittivity. Experimental findings are interpreted, for the first time, by means of a fully atomistic model that provides a novel microscopic interpretation of the observed Drude-Smith behavior.
Experimentally we have studied a thin polymer membrane, on top of which a graphene monolayer has been transferred. The sample is mounted on a mandrel with four clamps; by operating on the mandrel tightening mechanism, the sample can be strained. The sample is then analyzed with two spectrometers: a THz-TDS instrument, operating in the 0.3-2 THz spectral range, a FTIR instrument, operating either in the FIR (2-10 THz) or in the MIR (10-100 THz) spectral ranges depending on the employed beam-splitter and detector. The strain strongly affects the 0.3-2 THz region, while the 10-100 THz region is almost unaffected.
To interpret the observed spectra, we calculated by means of the multilayer scattering matrix method the trasmittance. The SM method employed here is the last "PPML" package available online from some of the authors[1]; its main input are the thicknesses of the layers and the conductivity of graphene. After an unsuccessful attempt to describe the graphene conductivity through a Drude model, we applied the Drude-Smith model, in its recent revision by Cocker et al.[2] This model quantifies the conductivity of a multi-domain conductor, a situation that may well describe our large-size poly-crystalline graphene sample. With this model we obtained a good agreement with experiments. We supported such explanation by a comparison with atomistic simulations relying on the wFQ approach[3], allowing a direct comparison with experimental results. In this scenario, the atomistic nature of wFQ is suitable for the description of cracks, bond elongations and the mutual motion of grain boundaries. Thus, wFQ can indeed model complex carriers transport in strained graphene. The physical parameters returned by wFQ are exploited to better interpret the meaning of Drude-Smith parameters, for which a microscopic interpretation is then given.

[1] https://it.mathworks.com/matlabcentral/fileexchange/55401-ppml-periodically-patterned-multi-layer
[2] Cocker, T. L. et al., Phys. Rev. B 96, 205439 (2017)
[3] Giovannini, T. et al., J. Phys. Chem. Lett. 11, 7595 (2020)

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