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Final report for the ESF-Exchange Visit Grant

The last four months had been a very fruitful time for me where I was able to work in a highly motivating environment. I have learned a lot of new interesting things and gained insight in several new aspects of plasmonics. This can also be seen by the huge amount of scientific output from this research visit: Two to three papers will be submitted in the next three months, the topics of two following articles had also been discussed and are part of my current work. Parts of my scientific output will be presented at the 12th international conference of Near-field Optics, Nanophotonics and Related Techniques (NFO) in San Sebastian in September 2012 and at other upcoming conferences.

During my visit, I was able to extend our MATLAB® toolbox MNPBEM, where we use the *Boundary Element Method (BEM)* to solve Maxwell's equations in the presence of arbitrarily shaped dielectrics. I have been working on several different topics; the two main parts were graphene plasmonics and nonlocal effects of metallic nanoparticles:

1. **Plasmons in Periodically Doped Graphene**
   Graphene plasmons can confine electromagnetic energy down to unprecedented small volumes, while exhibiting lifetimes greatly exceeding those of conventional metals for similar degree of confinement. Additionally, graphene plasmons are tunable through electrostatic doping, which provide a practical way for ultrafast electrical control of light fields. These excitations have been recently mapped and proved to have the expected degree of electrostatic tunability. Together with people from the group of Prof. García de Abajo I have been investigating graphene plasmon bands under periodic doping conditions, including the effect of inhomogeneous doping charges. We have been exploring the possibility of extreme subwavelength imaging resolution in a periodically doped graphene structure, as well as tunable levels of absorption towards external light. These results can find application to infrared sensing and spectral microscopy and will be presented at the NFO conference by Iván Silveiro.

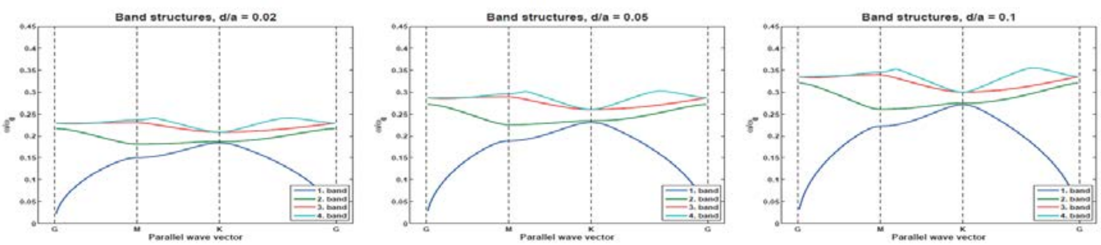

Fig. 1: First four band structures for a periodically doped graphene layer for different spacing and distances of the doping.

2. **Nonlocal Effects of metallic nanoparticles**
   The boundary element method which I am using for all my simulations is suited for homogeneous and isotropic dielectric environments, where the embedded bodies are separated by sharp boundaries. Especially when two particles get very close to each other (below 1 nm for example) or when the particles become very small, the neglect of nonlocal effects causes inaccuracies in the simulations. In

reality we do not have sharp boundaries because of the so called spill-out effect: Electrons are also on the outside of the metal surface. I have incorporated such effects by a simple method, where a new nonlocal dielectric function is used for the description of the metal, see Fig. 2.

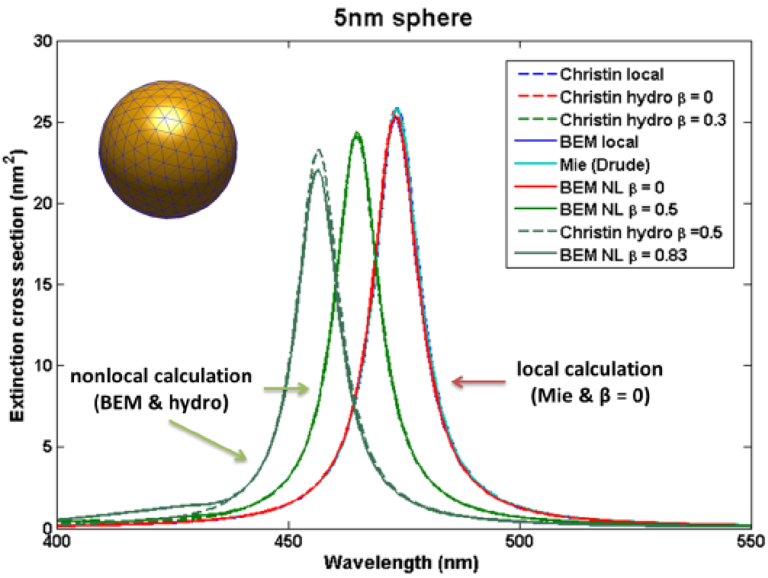

Fig. 2: Comparison of local and nonlocal spectra for a nanosphere with a diameter of 5 nm. The parameter β controls the amount of nonlocal influence and is connected to the Fermi wave vector of the material. My calculations show perfect agreement with the analytical solution for β = 0 and with different calculations for finite values of β.

A very big advantage of my work is that because of the BEM approach we are not restricted to spherical geometries anymore and we can calculate nonlocal effects for every particle shape. At the moment I am finishing some details and preparing the paper with the results. Parts of these results will be presented by Christin David again at the NFO conference and by me at several upcoming conferences. Since this method is a very suitable, fast and promising way for future calculations I have also already discussed the continuation of this work in close collaboration with Prof. García de Abajo.

3. Additional topics

At the moment I am also collaborating with the group of Prof. Kautek in Vienna, where I'm simulating the plasmonic fields of very long coated metal tips close to a metallic surface. These tips are approximately 4 µm long and because of memory limitations it is not possible to simulate them with the MNPBEM toolbox – I had to restrict the tip-length to a few hundreds of nm. But since the people in Madrid also developed a different simulation approach for such problems, I could confirm and certify my previous simulations with the MNPBEM toolbox.

During my stay I was also able to collaborate with a visitor from the McMasters University in Hamilton (Canada) from the Microscopy of Nanoscale Materials group headed by Prof. Gianluigi Botton. This group currently owns one of the best electron microscopes in the world and they are very interested in simulations of Electron Energy-Loss Spectroscopy (EELS), where a high-energy electron beam passes in the vicinity or through the nanoparticle. Some electrons lose energy through plasmon excitations, which are subsequently monitored. By raster scanning the beam over the metallic nanoparticle, one obtains information about the photonic local density of states of the metallic nanoparticles.
I was able to set up several BEM simulations which are in very good agreement with new experimental results from the Canadian group. Additionally I also succeed in combining EELS with the nonlocal approach discussed above, see Fig. 3.

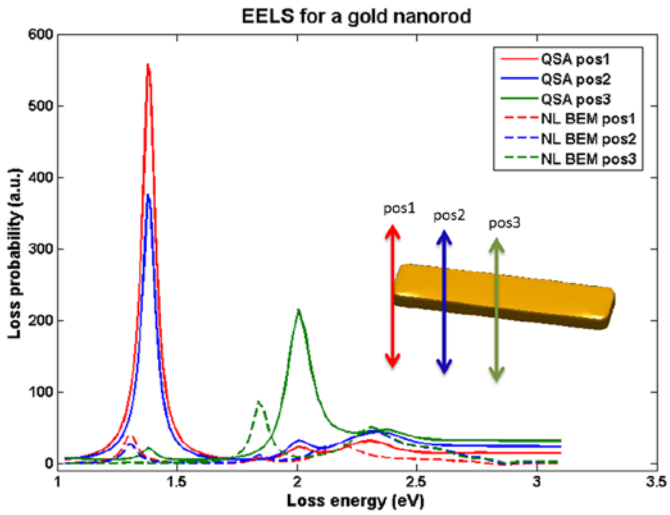

Fig.3: Comparison of local and nonlocal EELS spectra obtained from a simulation of a very flat and small nanorod with the MNPBEM toolbox. The different peaks correspond to the plasmon modes at the different electron beam positions indicated in the inset.

Because of the high spatial resolution of EELS measurements they allow the experimental investigation of very small particles or very small gap distances. Many research groups are already moving in this direction and because of my work we now already have a versatile simulation tool for such experiments at our hands.

In the end I gained a lot of insight and new ideas of how to solve several problems of my work and I had many fruitful discussions. The collaboration between me and the group of Prof. García de Abajo will continue and I want to thank the ESF committee for this great opportunity.

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