GRAPHENE: Graphene-Based Revolutions in ICT And Beyond

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We participate to the project Graphene-Based Revolutions in ICT And Beyond, GRAPHENE, Grant agreement number 604391CP-CSA, one of the most important initiatives in the European research. Among participants there are 23 Italian partners including research institutes, universities and enterprises, with 16 new partners including Istituto Nazionale di Fisica Nucleare represented by the NEXT group at LNF, led by Stefano Bellucci. Owing to the new partnerships the consortium binds together more than 140 organizations from 23 Countries, with the common aim of transfering graphene and related composite materials from academic laboratories to everyday applications.

The Graphene Flagship Project represents a European investment of 1 billion euro for the next decade and is part of the Flaghship Initiatives for future emerging technologies (TEF) announced by the European Commission in January 2013. Italy is already a leader in the development of important areas of the Graphene Flagship Project, including research in composite materials and energy applications, and it is involved in technology transfer and dissemination, as well. The participation of INFN is focused on the realization of multi-layered sandwich graphene devices, within the workpackage of high frequency applications.

Project objectives:

The main objective of the project is to investigate, both theoretically and experimentally, the shielding properties of artificial graphene-based 3D materials in the form of sandwiches alternating polymer films and graphene layers. The polymer thickness could vary between 100 nm to a few microns and the graphene can be composed of one to a few atomic planes. The sandwich can be both on substrate and free standing (and therefore flexible).

The electromagnetic properties of these sandwiches will be studied, not only in the radio-frequency (RF) domain, but also in the optical domain. For RF electromagnetic waves, the sandwich should roughly be equivalent to an effective polymer – graphite-like bilayer, where each layer has a thickness equal to the sum of the thicknesses that the same materials have in the sandwich. However, the electronic properties of the graphite-like effective medium will differ from that of bulk graphite. In the ultimate case where, in the sandwich, one-atom thick graphene is intercalated between polymer films, there will be no van der Waals coupling between the band structures of the individual graphene planes, due to their large separation distance, and the graphite-like effective medium will behave like 2D graphene, with however a thickness in the nanometer range. The same holds true if two or three graphene atomic planes are intercalated between the polymers films, except that the graphite-like effective medium will have the properties of a two- or three-plane graphite.

The possibility to tune graphene layers absorption-transmission characteristics by applying of electric fields, mechanical tension and acoustic waves for realization of switching shielding will be studied theoretically.

The temperature dependence of all EM material parameters (dielectric permittivity, AC conductivity at high frequencies – from MW to THz) for all produced GLM (graphene like materials) and graphene-based composites will be studied theoretically and experimentally.

Using self-consisted field equations describing the interaction of EM field with graphene electron

system we will estimate an optimal number of graphene layers at which EM absorption will be maximal for every MW and THz frequency range. The EM behavior of composites filled with GNP and other GLM will be modeled in microwave and THz ranges using "multi-physics" approach (together with LNF INFN), and nanoelectromagnetics combining classical electromagnetics and quantum properties of graphene nanomaterials.

Fundamental properties of graphene will be also studied as an added value: using THz/MW data on transmission/reflection through the graphene monolayers we can find such a fundamental characteristic of graphene as free path of π electrons.

Objectives of the workpackage High-Frequency Electronics

This workpackage is devoted towards the long term perspective of establishing graphene based highfrequency electronics technologies, which are capable of significantly outperforming state-of-the-art technologies. Therefore the key objectives of this WP are:

• Optimize process technologies critical towards meeting the requirements of specific applications, including work on contact resistance, gate stack, passivation, band gap engineering and integration of different 2D materials.

• Identify further key technological bottlenecks for realizing graphene based high frequency integrated circuits and develop solutions for solving them.

• Develop novel concepts for realizing graphene-based high-frequency devices including ballistic devices.

• Design and realization of graphene-based integrated circuits capable of fully utilizing the unique electronic properties of graphene.

• Develop new concepts for next generation radio-frequency micro-electro-mechanical systems (RF-MEMS) powered by graphene including novel bulk- and surface acoustic wave devices for wireless communications.

• Exploit the remarkable conducting properties of graphene to taylor efficient shielding coating layers that are compatible with the future HF electronics and may protect nanodevices against electromagnetic perturbations.

• Assess the developed technologies towards the current state-of-the-art and define target parameters

Technical progress in 2015

Microwave-photonic devices

With the increase in frequency range for technological application of graphene and its derivatives, the urge for ab initio methods to support semiclassical and multiphysics modeling is driving more and more attention. In particular, parameter-free and hybrid Density Functional Theory (DFT), Time Dependent (TD) DFT and Many-Body Perturbation Theory (MBPT), namely GW and Bethe-Salpeter Equation (BSE+GW), need to be considered. These are the most well established ab-initio techniques to compute structural, electronic and optical properties of finite (TDDFT) and extended (MBPT) systems as well as their interfaces on metal contacts or supporting substrates.

In particular the elctromagnetic behavior of extrinsic graphene and graphene-based nanomaterials, in terms of permittivity and conductivity response of the systems to applied electron and photon currents, is mostly investigated by tight binding (TB) approaches. The latter are interfaced with semiclassical transport models and nanocircuit analysis tools that are suitable for device-scale simulations. Furthermore, TB band calculations enter prominently in models of mechanical deformation and elastic

properties at the microscale level.

We have rececently set-up a self-consistent method based on a full wave approach, offered by TDDFT in linear response (LR) regime, which is capable of predicting the ab initio permittivity, conductivity and plasmon structure of mono and bilayer graphene at the atomistic scale [1-3]. Specifically, we have investigated the lower THz to IR features of the plasmon spectrum, where the dominant contribution is brought by the isotropic (linear) Dirac cone electrons, which are highly sensitive to doping. Nevertheless, special attention has been set on some outstanding anisotropic (non-linear) effects found for sufficiently high injected electron/hole densities. The main signature of this anisotropy in graphene is the occurrence of two distinct plasmon modes generated by carriers moving with different Fermi velocities along high-symmetry paths that originate at the Dirac points. Further anisotropic features are evident in the different electromagnetic behavior for positive and negative doping levels associated to Fermi energy shifts above 0.5 eV. The afore mention findings cannot possibly be predicted in the framework of TB approaches relying on the Dirac-cone approximation, simply because an oversimplified isotropic graphene band structure is considered in the vicinity of the Dirac-points. If confirmed by experiments, they will necessarily come into play in future nanodevice design.

<u>Microwave Devices</u>

The possibility to take advantage of the outstanding properties of graphene in the fabrication of devices suitable for microwave/RF applications depends on the quality of the actually produced samples. Severe performance hindering consequences may stem from fabrication defects and uncertainties, the presence of impurities, the effect due to grain boundaries, and in general the polycrystalline, rather than genuinely single crystal nature of the massively produced graphene specimens of industrial quality and economic viability, needed for fulfilling the promises of pure carbon consumer electronics.

At microwave/mm-frequencies, structures/devices require electric sizes of the order of the wavelength, while the size of the first available graphene samples was much smaller. However, graphene chemical vapor deposition (CVD) nowadays allows one to obtain samples up to several centimeters, thereby increasing the research interest for the realization of passive devices at such frequencies having at hands several optimization parameters, including gas flowing rate, temperature, pressure, deposition time Then, even if graphene in the microwave/mm range behaves as a moderate conductor, it still preserves the outstanding property of tunability, that consists in the possibility to electrically induce electrons or holes (e.g., by applying a positive or negative voltage), thus leading to the tuning of its resistance.

Graphene Microstrip Attenuator

A broadband microstrip attenuator, operating in the frequency band from 1 GHz to 20 GHz and based on few layer graphene (FLG) flakes, was introduced in [4].

The circuit consists of a 50 micron microstrip line with a gap, where the FLG is located (Fig. 1a). To guarantee a better contact deposition of the FLG, the terminal open ends of the microstrip lines are cut with 45° slope. Two bias tees are used to properly bias the graphene with the desired voltage across the gap. By changing the value of the bias voltage applied to the graphene, the surface conductivity of graphene can be modified, and consequently the insertion loss of the microstrip attenuator can be electronically tuned.

A prototype of the graphene-based microstrip attenuator was fabricated to verify its electromagnetic performance and tunability. The manufacturing of the circuit was performed by using a LPKF micromilling machine, able to define the desired shape of the microstrip lines and the slope of the open ends. The photograph of the adopted measurement setup is shown in Fig. 1b.



Fig. 1 Graphene-based microstrip attenuator: (a) geometry of the measurement setup; (b) photograph of the prototype in the measurement setup; (c) measured insertion loss vs. frequency, for different values of the bias voltage (from [4]).

The measured insertion loss of the attenuator over the frequency range from 1 GHz to 20 GHz is shown in Fig. 1c, for different values of bias voltage across the gap. As expected, the insertion loss can be significantly modified by the applied voltage. The insertion loss increases with frequency, but a tuning of the insertion loss with the bias voltage is evident over the entire frequency range. In particular, a larger tuning range can be achieved at lower frequency (approximately 5.5 dB tuning at 1 GHz), while smaller values down to 2.5 dB are achieved at the frequency of 20 GHz. The maximum usable tuning voltage is 5.5 V, as higher values lead to a permanent damage of the attenuator, due to the large current flowing through the graphene pad [4].

[1] Mencarelli, D.; Bellucci S.; Sindona, A; Pierantoni, L. Spatial dispersion effects upon local excitation of extrinsic plasmons in a graphene micro-disk, Journal of Physics D: Applied Physics, Volume 48, Number 46, Published 20 October 2015

[2] Sindona A.; Pisarra M; Mencarelli D; Pierantoni L; Bellucci S. Plasmon modes in extrinsic graphene: ab~initio simulations vs semi-classical models, in Fundamental and Applied Nano-Electromagnetics, Maffucci, A; Maksimenko, S. A. (Eds.); 2016 Springer

[3] Pisarra, M.; Sindona, A.; Riccardi, P.; Silkin, V. M.; Pitarke, J. M. Acoustic plasmons in extrinsic free-standing graphene New J. Phys. 2014, 16, 083003; (38) Pisarra, M.; Sindona, A.; Gravina, M.; Silkin, V. M.; Pitarke, J. M. Dielectric screening and plasmon resonances in bilayer graphene Phys.

Rev. B 2016, 93, 035440.

[4] L Pierantoni, D Mencarelli, M Bozzi, R Moro, S Moscato, L Perregrini, F Micciulla, A Cataldo, S Bellucci, Broadband microwave attenuator based on few layer graphene flakes, IEEE Transactions on Microwave Theory and Techniques, 63 (8), 2491-2497 (2015)

List of Conference Talks by LNF Authors in the Year 2015

S. Bellucci, Graphene materials for electronic and electromagnetic applications, 27th Indian-Summer School on Graphene - the Bridge between Low- and High-Energy Physics, September 14 - 18, 2015, in Prague, Czech Republic.

S. Bellucci, Electromagnetic characterization of graphene and graphene nanoribbons via ab-initio permittivity simulations, Is quantum theory exact? The endeavor for the theory beyond standard quantum mechanics. Second Edition FQT2015, INFN-LNF, Frascati (Italy), Sept. 23-25, 2015

S. Bellucci, Ballistic Ratchet effect on patterned graphene, FM&NT-2015 | Functional Materials and Nanotechnologies, Vilnius (Lithuania), 5-8 October 2015

S. Bellucci, Electrical conductivity of graphene: a time-dependent density functional theory study, Semiconductor Conference (CAS), 2015 International, Sinaia (Romania) 13 - 15 October 2015.

S. Bellucci, Excitation of surface waves at terahertz frequencies on a suspended graphene sheet, 2nd Bilateral Indo - Italian Workshop October 11-14, 2015 NEEM2015 CNR Roma (Italy).

S. Bellucci, What Next in Condensed Matter, INFN-LNF, Frascati (Italy), Feb 27, 2015.

S. Bellucci, Research Seminar, Unical Cosenza (Italy), 10 March 2015

S. Bellucci, Broadband electromagnetic response and applications of graphene related materials, NATO Advanced Research Workshop on Fundamental and Applied NanoElectroMagnetics, FANEM 2015, Minsk, Belarus, May 25-27 2015

S. Bellucci, Electromagnetic characterization of graphene and Graphene nanoribbons via ab-initio permittivity simulations, International Conference on Electromagnetics in Advanced Applications (ICEAA 2015), Turin (Italy), Sept. 7-11, 2015

A. Maffucci, Synthesis and electrical characterization of graphene nanoplatelets, Electromagnetic characterization of graphene and Graphene nanoribbons via ab-initio permittivity simulations, International Conference on Electromagnetics in Advanced Applications (ICEAA 2015), Turin (Italy), Sept. 7-11, 2015

Publications by LNF Authors in the Year 2015

1. Electromagnetic characterization of graphene and graphene nanoribbons via ab-initio permittivity simulations, S Bellucci, A Sindona, D Mencarelli, L Pierantoni, 2015 International Conference on

Electromagnetics in Advanced Applications (ICEAA), 926-929, Editor IEEE.

2. Synthesis and electrical characterization of Graphene Nanoplatelets, A Maffucci, F Micciulla, A Cataldo, G Miano, S Bellucci, 2015 International Conference on Electromagnetics in Advanced Applications (ICEAA), 301-304, Editor IEEE.

3. Applications of Graphene at Microwave Frequencies, M. Bozzi, L Pierantoni, S Bellucci, Radioengineering 24 (3), 661 (2015).

4. Broadband Microwave Attenuator Based on Few Layer Graphene Flakes, L Pierantoni, D Mencarelli, M Bozzi, R Moro, S Moscato, L Perregrini, F. Micciulla, A. Cataldo, S. Bellucci, IEEE Transactions on Microwave Theory and Techniques, Aug. 2015, vol. 63, no. 8, p. 2491–2497. DOI: 10.1109/TMTT.2015.2441062.

5. Spatial dispersion effects upon local excitation of extrinsic plasmons in a graphene micro-disk, D Mencarelli, S Bellucci, A Sindona, L Pierantoni, arXiv preprint arXiv:1507.07090661 Journal of Physics D: Applied Physics Volume 48, Number 46, Published 20 October 2015 (2015).

6. M. Baldelli, L. Pierantoni, S. Bellucci, Learning by Using Graphene Multilayers, IEEE Microwave Magazine (Volume:17, Issue: 1), pp. 44 – 51, Date of publication: 10 December 2015