Microwave and optical bioelectrodynamics at the nanoscale and molecular level

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Summary: Here we focus on selected topics at the molecular level of how electromagnetic field is generated within organisms and how organisms can be affected by electromagnetic field. In the first part, we present our recent contributions to research microwave dynamics and interactions on nano- and biomolecular scale. We show in theory that a resonant MW coupling to nanostructure vibrations in liquid is possible, in contrast to what was previously thought, when the liquid slips at the nanostructure surface. Then we summarize microwave properties of biologically ubiquitous nanostructure – microtubules and describe rational design of the chip for microvolume dielectric spectroscopy. Our results contribute to fundamental insights into the dynamic behavior of matter at the nanoscale and new techniques in MW biosensing. In the second part, it will be explained how reactive oxygen species formed in cells and biomolecular systems generate ultra-weak photon emission and how this photon emission can be measured and exploited for non-invasive and label-free monitoring of oxidative processes and stress.

Introduction: Elucidating the physical and chemical parameters that govern interaction of electromagnetic field at the nanoscale and molecular level of matter is important for understanding the behavior of matter. Here we employ molecular dynamics, coarse-grained and analytical theoretical approaches to understand electromagnetic properties of biomolecules and nanostructures in microwave band and show how to rationally design a sensing chip based on the structure of biomolecule to be analyzed. We also explain the current understanding on how the organisms generate electromagnetic field in the optical band.

Results and Discussion: We developed an analytical model of microwave absorption of a longitudinally oscillating and electrically polar rod-like nanoresonator embedded in a viscoelastic fluid [1]. We showed that the slip length, which can be tuned via surface modifications, controls the quality factor and coupling of nanoresonator vibration modes to microwave radiation. We demonstrated that the larger slip length brings the sharper frequency response of the nanoresonator vibration and electromagnetic absorption, see Fig. 1. We showed in several works that microtubules, essential components of biological cell and necessary for cell division, have their normal vibration modes in MHz and GHz region [2,3] which can generate local electromagnetic field at the same frequency range due to microtubule polarity, see Fig. 2.

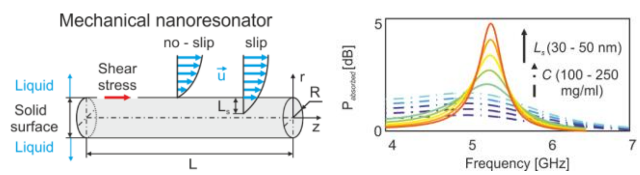

Fig. 1. Left Schematic illustration of fluid flow around a longitudinally vibrating cylindrical nanoresonator of length L and radius R. The slip boundary condition enables a non-zero velocity of the fluid at the nanoresonator surface. **Right** In bulk solution, higher concentrations of nanoresonators (C = 100 - 250 mg/mL with 10 nm slip length, dashed line) yield increased microwave absorption around the resonant frequency. The slip length (L_s = 30 - 50 nm with 250 mg/mL concentration, solid line) increases the sharpness of the microwave absorption frequency response. The data here regards a 500 nm long nanoresonator with a 500 $\mu C/cm^2$ surface charge density. Adapted from [1].

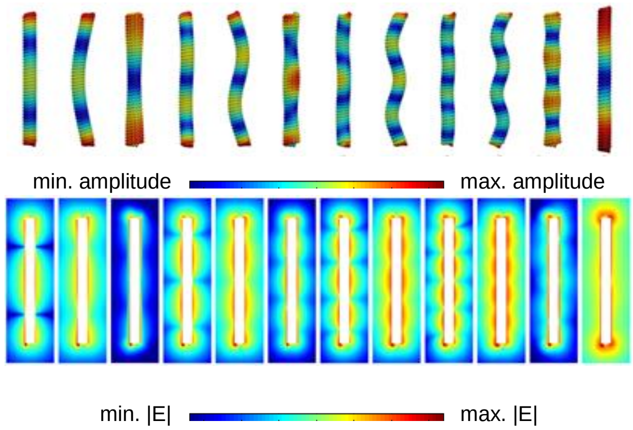

Fig. 2. Up Vibration mode pattern, **Down** electric field pattern of 320 nm long microtubule (white rectangle). First 12 nonzero modes (7-18) displayed with the mode frequency.

Recently we proposed a sensing microwave chip and evaluated its performance using both an analytical model and electromagnetic simulator [4]. We designed and fabricated the chip and experimentally demonstrated that we can extract the complex permittivity (0.5 - 40 GHz) of the water solution of alanine with about 20-fold smaller volume than with commercial methods. We also explored the role of a molecular model of water since it is the major compound determining microwave dielectric properties of biological tissues and wet samples. We analyzed how the common molecular water models (SPCE, TIP3P, and TIP4P) affect complex permittivity of biomolecular solutions predicted by molecular dynamics simulations. We found that the type of the molecular water model used in the simulation affects not only water contribution but also biomolecule contribution to the permittivity spectra.

Biological systems continuously generate a light (visible band electromagnetic radiation) of ultra-weak intensity. Recently we performed series of works to understand generating mechanism of this light [5]: Organisms endogenously produce a small amount of reactive oxygen species (ROS) in the course of their normal metabolism and in an enhanced manner when they undergo stress. A reaction of ROS with biomolecules leads to the formation of, apart from other products, unstable biomolecular intermediates such as dioxetanes and tetraoxides which can produce excited electron species when decomposed. The primary electron excited species considered to be generated are the triplet excited carbonyls and singlet oxygen. Excitation energy can also be transferred to energy acceptor to produce secondary electron excited species. If not deactivated or quenched, these excited states decay radiatively via emission of photons. Therefore, although through a chain of events, the intensity of photon emission reflects a rate of oxidative processes ongoing in the organism. This connection suggests that detection and analysis of the endogenous biological chemiluminescence (EBC) could be used to monitor oxidative processes in a non-invasive and label-free manner.

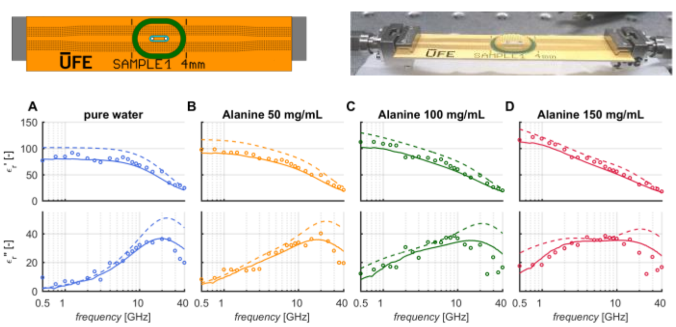

Fig. 3. Up The designed chip. **Down** Real and imaginary parts of relative complex permittivity of a liquid specimen obtained using our chip (circles) vs. reference coaxial probe bulk measurement (solid line) and from molecular dynamics simulation (dashed line) for A) pure water, B) 50 mg/mL, C) 100 mg/mL, and D) 150 mg/mL of alanine concentration in the water. Adapted from [4].

Refercnces:

[1]. O. Krivosudský, and M. Cifra. "Microwave absorption by nanoresonator vibrations tuned with surface modification." EPL (Europhysics Letters) 115.4 (2016): 44003
[2] D. Havelka, M. Cifra, and O. Kučera. "Multi-mode electro-mechanical vibrations of a microtubule: In silico demonstration of electric pulse moving along a microtubule." Applied Physics Letters 104.24 (2014): 243702.
[3] O. Kučera, D. Havelka, and M. Cifra. "Vibrations of microtubules: Physics that has not met biology yet." Wave Motion 72 (2017): 13-22
[4] D. Havelka, O. Krivosudsky, J. Prusa, and M. Cifra. "Rational Design of Sensor for Broadband Dielectric Spectroscopy of Biomolecules." *Sensors and Actuators B: Chemical* 273C (2018): 62–69
[5] M. Cifra and P. Pospíšil. "Ultra-Weak Photon Emission from Biological Samples: Definition, Mechanisms, Properties, Detection and Applications." *Journal of Photochemistry and Photobiology B: Biology* 139 (2014): 2–10

Info about speaker:

Dr. Michal Cifra, since **2013** head of **Bioelectrodynamics** research team (Institute of Photonics and Electronics, Czech Academy of Sciences). **PhD 2009, Radioelectronics**, (Czech Technical University in Prague, Czechia), **Ing. (M.Sc.) 2006, Biomedical Engineering** (University of Žilina, Slovakia). Apart from ~**1 year** biophotonics research experience from **Germany (RWTH, Aachen / IIB, Neuss)**, he also gained experience with high frequency bioelectronic interfaces (**8 months, University of Chicago, USA**).

His **long term vision** is to explore novel paths to future electrodynamic and electronic therapeutic and diagnostic methods in biotechnology and medicine. To fulfil the vision, he and his team develop computational methods and nanotechnology enabled experimental tools to analyze both active and passive electromagnetic properties of biomaterials from the level of molecules to tissues.

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Laboratory website and link:

http://bioed.ufe.cz/

https://twitter.com/BioED_IPE

Link to talks:

Electromagnetic activity of cells from spectral perspective, 2016

https://owncloud.cesnet.cz/index.php/s/Nqz15FgzMGNTlu0

Light of living organisms – in Czech, 2016

http://tydenvedy.msite.cesnet.cz/Mediasite/Play/49494118929548bc9f66aa0d6bbc630e1d?catalog=1e79760d-8359-4ee4-88a6-b4e264249e54

Light of living organisms – in Slovak with English subtitles, 2012

https://www.youtube.com/watch?v=gezEio1mdjs