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Study of electromagnetic spectrum of nano-sized viral particles via simulation

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Study of spectral characteristics of nano-sized viral particles, virions the extracellular infective forms of viruses is proposed. Morphology of virions is icosahedral, prolate or helical, size of that varies from 20 to 300 nm. Based on structure analysis of virions, consisting of inner core of nucleic-acids (RNA or DNA) and outer protective protein coat (capsid), the core-shell model of virus-like particle (VLP) is considered for simulation.

The single-particle study of electromagnetic (EM) wave & VLP interaction is based on Maxwell EM theory, separation of variables method for solving Helmholtz equation. Theoretical solution of electrodynamics boundary problem is applied for determination of EM fields in the areas of core, shell and surrounding medium of nano-sized particles. EM fields are presented as the sum of multipole wave-modes, number of that depends on "electrical" size of particles and is defined empirically within prescribed accuracy. Expected spectral "response" is observable on far-field characterizations and strongly depends on core-shell related electric and geometric parameters of VLP, especially in resonance wavelength range.

Computer simulation (based on MatLabR2013b) is used for studying EM field characteristics vs excitation wave length, for appreciation of possible resonant wave range correlating with scattering efficiency of VLP. VLP "spectrum" is demonstrated for cylindrical nanoparticle, namely un-enveloped rod-like virion of Tobacco Mosaic Virus (TMV), deciding 2D boundary problem.

Proposed methodology for modelling of EM spectra of virions seems to be a simpler way in determining the spectral response of whole viral particle, which in complement with experimental spectroscopic studies could solve the problem of defining the unique and specific "fingerprints" important in nano-bio-particles characterization. Findings are applicable in nano-bioparticles detection and identification systems, aerosol spectroscopic studies as well.

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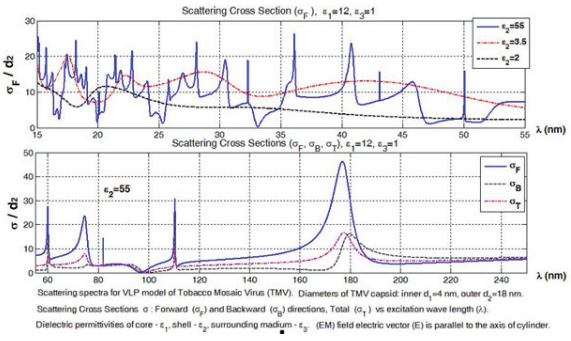

Speaker Biography

Tamar Bzhalava is an associate professor at the Department of Engineering Physics, Georgian Technical University (GTU). She was the candidate (PhD) of Physics and Mathematics Sciences (1990). She was the scientific manager (2014-2017) of grant project of Shota Rustaveli National Science Foundation (SRNSF) - "Nano-Sensory Applications for Studying-Elaboration of Detecting Model of Pathogenic Microorganisms". She is the member of scientific team elaborated successful international and local Scientific Projects: SENS-ERA, FP7-INCO-2011-6 (2013); International Science and Technology Centre (ISTC) grants (2006-2009, 2003-2004); Georgia National Science Foundation (GNSF) grant (2006-2008). She has been a participant and member of organizing committees of international and national scientific conferences, workshops. She is an author up to 70 scientific publications, text books, Principle of Master Program at GTU. Her research interests mainly focus on oscillation, scattering, spectral properties of nano-micro-particles, EM-wave & particles interaction, applied electrodynamics, teaching general physics, modeling, simulation.

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