RESPONSE

of the official opponent on the PhD work

"Diffraction radiation from dielectric, silver and graphene circular nanowire configurations excited by modulated electron beam", authored by Dariia O. Herasymova and presented for defense on the degree of Doctor of Philosophy in specialty 104 – Physics and Astronomy

Relevance of the dissertation topic

The moving charged particles, such as electrons, radiate the electromagnetic waves passing through the boundary between the material media. Such effects termed as the transition or the Cherenkov radiation. The radiation of electrons moving in vacuum without crossing any material boundaries has also attracted the attention of researchers since 50-ies of the last century. The most known example of such effect is the Smith-Purcell radiation, which is associated with an electron beam flowing through a periodic array, for instance, ruled on a metal surface, across the grooves. In this concern, the Smith-Purcell effect is only a particular case of more general phenomenon that is radiation of the surface; and the polarization currents induced on the metal and dielectric objects by the electron beams flowing in their vicinity do not touching them. This type of electromagnetic-wave radiation is usually termed as the diffraction radiation.

Microwave-range of diffraction radiation is already used as a convenient method for non-invasive diagnostics of beams in accelerators, namely for remote sensing of the position and velocity of the particle (electron) beams. Such devices are usually referred as the beam position monitors. The development of such devices can be extended to the optical range, because the emergence and rapid development of nanotechnology opens the way to create ensembles of nanosize optical scatterers with the controlled shape and location. Nanoscale components introduce very little perturbation to the beam, its velocity and trajectory, and therefore its field can be fixed. Therefore, the analysis of the diffraction radiation effect can be performed within the classical theory of electromagnetic wave scattering, i.e. as the scattering of wave by the objects of known shape and material parameters. Many problem in this field are does not investigated yet, therefore study of radiation from dielectric, silver and graphene circular nanowires and array consisting of such wires is actual problem in both the theoretical and engineering relation.

The structure and content of the work

The dissertation consists of abstracts, an introduction, five chapters that contain 73 figures, conclusions, a list of used sources with 159 titles and an appendix. The total volume of the dissertation is 175 pages.

Introduction is focused on the justification of the choice of research topic, specification of the object of research, explaining the research goals and problems, justification of the research methods, accentuation of scientific novelty of obtained results and practical worth of obtained results, specification of personal contribution of the author, presentation of the research results at the scientific international conferences, and confirmation of the relation of the thesis' topic to scientific research of Institute, where the thesis was prepared.

The **first chapter** is devoted to literature review and specification of the research methods applied for the investigation. Author focuses on the methods of analysis of wave scattering from circular dielectric cylinders, the recipes how the field of a harmonically modulated beam of charged particles can be presented, description of properties of the complex permittivity of silver material as a function of frequency, introduction to the graphene and its characteristics using the Kubo formalism, specification of scattering and absorption cross-sections and optical theorem, and explaining the necessity of research related to lasing eigenvalue problem.

Author considers the diffraction radiation of a beam of particles moving near dielectric nanowires in the **second chapter**. The diffraction radiation scattering and absorption characteristics in the visible frequency range for a single circular dielectric nanowire and dimer of twin circular dielectric nanowires excited by the modulated electron beam are explained here. The semi-analytical technique, which exploits the Fourier expansions in the local coordinates of each wire and the addition theorems for the cylindrical functions, is used for solving the problems. Using such approach, author studies a single dielectric wire's resonance diffraction radiation fields and identifies them as the linear combinations of two degenerated modes of a circular cavity. It was shown that for the dimer the modes are the supermodes, and they are built on the natural modes of the constituent dielectric cavities combined together and obey to the two-fold symmetry. To justify the above relations, author studies the scattering problem formulation for finite number of circular wires, explains the mechanism of reducing the problem to the Fredholm 2-nd kind matrix equation, studies the resonances on whispering gallery modes for single dielectric nanowire, explains how two dielectric nanowires can be used as a model of beam position sensor, and provides comprehensive numerical modelling related to resonances on the dimer supermodes.

The **third chapter** is devoted to diffraction radiation of a beam of particles moving near the silver nanowires. The diffraction radiation scattering and absorption characteristics in the visible range are numerically investigated in this chapter for a stand-alone circular silver nanowire and twin circular silver nanowires and nanotubes. Such configurations are investigated applying the Beam Position Monitor applications. The wavelength-dependent permittivity of silver is adopted from the experimental data and demonstrates the negative real-part values. Owing to this fact, sub-wavelength in radius silver nanowires is famous as nanoresonator due to the localized surface-plasmon modes. Author uses the field expansions in the form of azimuth Fourier series, and the addition theorems for the cylindrical functions, similarly to chapter 2. Such approach allows to get the solution of the one-wire problem analytically and to reduce it to a Fredholm second kind infinite-matrix equation for silver-wire and silver-tube dimers. The convergence of numerical solution is confirmed by the Fredholm theorem.

The developed in the previous chapter approach is extended for research of the diffraction radiation of a beam of particles moving near graphene-covered dielectric nanowires in **chapter four**. It is assumed that the beam velocity is fixed, and the separation of variables in local coordinates and the addition theorems for cylindrical functions to reduce the diffraction radiation problem to a Fredholm second-kind matrix equation are used. The twoside resistive boundary conditions are applied for zero-thickness graphene covers. The electron conductivity and as a result, the surface impedance of grapheme, are determined using the Kubo formalism. A great attention is paid to the resonances on the lattice modes for finite array of graphene-coated nanowires. The theoretical results are supported by the numerical simulation, related to study of the resonances on the plasmon supermodes and diffraction radiation effects for finite graphene-covered nanowire array.

In **chapter five**, the previous results are used for substantiating the threshold conditions for single and twin graphene-covered quantum nanowire lasers. The implementation of the lasing eigenvalue problem approach for study of the electromagnetic field in the presence of a circular quantum wire made of a gain material and wrapped in graphene cover, and a dimer of two identical graphene-covered quantum wires at the threshold of stationary emission, is realized here. The lasing eigenvalue problem approach allows to extract the mode-specific eigenvalue pairs, namely the frequencies and the threshold values of the quantum wire gain index for the plasmon and the wire modes of such nanolasers. As in the previous chapters, author uses the quantum Kubo formalism for the graphene conductivity and classical Maxwell boundary-value problem for the field functions. The numerical results on the full-wave analysis of single-wire laser mode properties and the dimer-wire laser mode properties confirm the effectiveness of the approach proposed.

The **conclusions** of the work are clearly formulated; they fully highlight the results obtained in the work. In terms of their content and level of argumentation, the conclusions meet the requirements for dissertations for obtaining the scientific degree of Doctor of Philosophy.

The **reference list** is informative; it characterizes comprehensively the research field under investigation and demonstrates the author's extensive erudition in this field.

The degree of validity of scientific statements, conclusions and recommendations, their reliability

The author of the dissertation performed an analysis of a specific problem of researching the scattering of electromagnetic waves by dielectric, silver and graphene nanowires, carried out a comprehensive theoretical and practical justification of ways to solve it. The validity and reliability of the scientific results, conclusions and recommendations presented in the dissertation work are achieved by using the justified methods of solving the scattering problems on a set of nanosize bodies and a thorough multi-faceted systematic analysis of physical processes in a set of such wires using the results of numerical modeling.

The novelty of the scientific statements of the dissertation work

In the process of studying the diffraction radiation effects for various configurations of circular nanowires and nanotubes made of dielectric, silver, and graphene excited by the modulated beam of charged particles, based on the goal of the work, the author obtained a series of new scientific and practical results, among which, in my opinion, the most important are the following:

1. It is substantiated that the beam trajectory is shifted from the central (symmetric) position between the twin nanowires, the diffraction radiation scattering and absorption spectra demonstrate the appearance of previously unknown resonances, associated with the dimer supermodes whose fields are orthogonal, and the intensities of new peaks are proportional of the beam displacement or its angular shift.
2. In the process of the diffraction radiation analysis for the sparse finite periodic arrays of many graphene-covered nanowires it is shown by computations that the dominant feature in the frequency spectra of diffraction radiation power defines the resonances on the plasmon modes of each wire and the lattice modes of the whole array.
3. Analysing the lasing threshold conditions of the modes of single circular graphene-covered active wire, author substantiated that if the wire radius is larger than 10 μm, then the "parasitic" dielectric wire modes are not weaker that the "working" plasmon modes relatively to the frequencies and in the threshold values of the gain; the above is important information for the practical implementation of the corresponding arrays.

Practical worth of the obtained results

The practical significance of the obtained results lies in the possibility of using the results of numerical modeling for the development of plasmonic graphene nanolasers.

The developed software for studying the scattering and absorption characteristics of the nanoarrays can be used as platform for numerical optimization of optical devices, key elements of which are circular nanowires.

The main results of the work have been published in 25 scientific works, 6 of them have been published in the international scientific journal belonging to Q1 – Q2 quartiles, 19 publications are materials of international scientific conferences cited in Scopus.

Approbation of the results of the dissertation work. The obtained research results have sufficient approbation, which is confirmed by the presentations at the prestigious international scientific conferences, in particular,

- European Microwave Conferences (EuMC), Paris (2019), Utrecht (2020), London (2021), Milan (2022), Berlin (2023);
- IEEE International Conference on Microwaves, Communications, Antennas, and Electronic Systems (COMCAS), Tel Aviv (2019);
- European Conferences on Antennas and Propagation (EuCAP), Copenhagen (2020), Madrid (2022), Florence (2023);
- EEE/MTT-S International Microwave Symposium (IMS), San Diego (2023).

Remarks

1. In page 9, Annotation in Ukrainian, the first item of the scientific novelty, the third line, the word "відсутні"must be replaced by "невідомі".

2. This remark follows from the previous one, namely, in page 22, the first item of the scientific novelty, third line, the word "absent" is used incorrectly, must be used "unknown" instead of.

3. In the last item of scientific novelty (page 23, the second paragraph below), where is said about the threshold of supermodes for the stand-alone and set of wires, it is declared that

the threshold values can be differ, but this is not demonstrated convincingly by the numerical simulation.

4. The numerical results are widely presented, but the quality of figures requires the higher resolution, because of quantitative assessment of the radiation characteristics is inconvenient (this concerns to Fig. 2.5, Fig. 2.6, and so on).

5. In pages 67-68, it is said that the Optical Theorem has been satisfied at the level of machine precision and the boundary conditions have been satisfied with the same accuracy as the solution of the matrix equation (2.36), but there no numerical data concerning this statement. In my opinion, such numerical data would be a strong confirmation of the analytical statements that relate to this provision.

Summarizing, one should note that the above-mentioned remarks related to drawback of dissertation do not affect the overall positive assessment of the completed research; they do not reduce the scientific novelty and practical worth of the dissertation work, and do not reduce the overall positive assessment of the conducted investigations.

Conclusion

Ph.D. dissertation “Diffraction radiation from dielectric, silver and graphene circular nanowire configurations excited by modulated electron beam”, authored by Dariya O. Herasymova written in modern scientific and technical language, consistently, logically and competently. The style of presentation of the material ensures accessibility of its perception. Dissertation work in terms of content is a completed scientific study containing new scientifically based results that are important at the current stage of studying the scattering characteristics of the nanowires and arrays consisting of such nanowires, and it corresponds to the fields of investigation in the specialty 104 – Physics and Astronomy.

The scientific worth of the dissertation is undoubted, because the results of research are published in six papers of the journals, which belong to Q1 – Q2 quartiles. In terms of scientific level, practical worth, approbation and publications, the dissertation meets the requirements set forth in the Order of the Ministry of Education and Science of Ukraine on January 12, 2017 No. 40 "On Approval of Requirements to Design of Dissertation" and also meets the requirements stipulated in Clause 10 of the "Procedure for Conducting the Experiment on Awarding the Degree of Doctor of Philosophy" and approved by Resolution of the Cabinet of Ministers of Ukraine on March 6, 2019 No. 167 "On Conducting an Experiment on Awarding the Degree of Doctor of Philosophy", and its author, Dariia O. Herasymova deserves to be awarded with the scientific degree of Doctor of Philosophy in the field of knowledge 10 "Natural Sciences" with specialty 104 – “Physics and Astronomy”.

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February 01, 2024

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