Introduction

Nanophotonics examines the interaction of light with particles of matter or irregularities that are smaller and much less than the wavelength, and devices produced on the basis of the results. Nanophotonics in particular includes the optics of photonic crystals and photonic-crystal waveguides, plasmonics, near-field microscopy, metamaterials and optical micromanipulation.

According to the wave-particle duality, the light during its propagation (except for acts of emission and absorption) can always be considered as a wave. Even if the number of photons is small (very weak light fields) we can observe phenomena of diffraction and interference. Therefore, Maxwell's equations always adequately describe the propagation of light – interference and diffraction in free or homogeneous space.

The interaction of light with matter is described by macroscopic or microscopic electrodynamics. In *macroscopic electrodynamics* Maxwell's equations the matter is described by dielectric and magnetic permeability, charge density and the current density vector of charges; the absorption of light is described by the introduction of complex dielectric permittivity material. *Microscopic electrodynamics* is based on Maxwell–Lorentz equations. These equations are a generalization of Maxwell's equations, in which matter is described as a set of moving point charges. According to the electron theory, the Maxwell–Lorentz equations accurately describe the electromagnetic microfields any point in space (including the inter- and intratomic fields and even fields inside elementary particles) at any time.

Adequate microscopic description of the emission, absorption, and scattering of light by material is provided by quantum electrodynamics. *Quantum electrodynamics* quantitatively describes the effects of the interaction of radiation with matter, and also consistently describes the electromagnetic interaction between charged particles. *Diffractive nanophotonics*, which is the subject of this book, deals with the processes and devices in which the wave properties of light are predominant. Diffractive nanophotonics suggests the possibility of describing the processes of behaviour of light by the Maxwell equations. The Maxwell equations can be used when working with coherent electromagnetic fields. In this case, the characteristic dimensions of the optical elements and structures should significantly exceed the atomic size. This is necessary to describe

the optical properties with the macroscopic characteristics of dielectric permittivity and magnetic permeability. Thus, diffractive nanophotonics studies light diffraction on macro-objects with minimal irregularities of the order of tens of nanometers, up to the quantum dots of about 10 nm in size (this is much larger than the size of individual atoms and simple molecules of the substance). Therefore, the substance is described at the macrolevel, i.e. in the framework of macroscopic electrodynamics. The limitation is that in diffraction of light on free micro- and nanoinhomogeneities (e.g., solid microparticles in fluids), light presses on microparticles with a force of units and tens piconewtons and makes them to move. Thus, strictly speaking, it is required to solve the non-stationary problem of the diffraction of light on a moving heterogeneity and take into account the change in the wavelength of light.

The main purpose of this book is to demonstrate the fruitfulness of the well-established methods of diffractive computer optics in solving nanophotonics tasks. There are 8 chapters and 3 appendices in the book.

In the first chapter the basic equations of the diffractive nanophotonics and related transformation are considered. A system of Maxwell equations is presented and the formulation of the conditions on the interfaces and the Poynting theorem is discussed.

The basic equations that can be obtained from the system of the Maxwell equations are presented. These include the wave equation (with the time dependence of the field), the Helmholtz equation (without such dependence), the Fock–Leontovich equation (approximation of the scalar diffraction theory) and the eikonal equation and transfer (ray tracing approach). The integral theorems of optics expressing the field values in the integral form are presented. These include the Green (scalar case) and the Stratton–Chu (vector representation) formulas. The scalar integral transforms are considered for use in optics to calculate the diffraction field in a homogeneous space: the Kirchhoff integral corresponds to the decomposition of the complex amplitude of the field in spherical waves, the Fresnel integral – along parabolic, and the Fourier transform – for plane waves.

The second chapter is devoted to numerical methods for solving diffraction problems under the strict electromagnetic theory. The first section presents difference method for solving Maxwell's equations (FDTD approach). The Yee explicit difference schemes, based on the replacement of the difference derivatives by relationships for grid functions are discussed. In addition, each projection of the electromagnetic field is defined by its grid domain, which improves the order of approximation of the differential problem. The method of transition from grid functions in space and time to complex amplitudes of the field components is developed. Particular attention is given to the imposition of absorbing layers, simulating the free space around the computing domain. The problem of the formation of the electromagnetic wave incident on the optical element is solved. A method is proposed for the decomposition of the grid area, allowing a

large reduction of the duration of calculations by taking into account the structure of the optical elements. The second part of this chapter deals with approaches to numerical solution of the Helmholtz equation. A review of existing approaches is given and their classification in the family of BPM methods (beam propagation method) discussed, and the principal differences between the different versions of the method are shown. The solutions of the scalar Helmholtz equation for paraxial cases (in the approximation of the smooth envelope) and non-paraxial (based on the approximation of the differential operator) distribution are presented. The finite-difference schemes for solving equations and boundary conditions for some variants of the boundary conditions are given. Approaches to solving the Helmholtz equation for the vector case are discussed, including the media with an inhomogeneous distribution of the refractive index.

The third chapter examines the diffraction of light on two-dimensional microscopic objects of arbitrary shape. The problem of diffraction of electromagnetic waves with TE or TM-polarization on two-dimensional dielectric objects is solved using the finite element method (FEM) in different conditions. The Helmholtz equation is solved by the combined Galerkin FEM and the boundary element method. Two types of this method are considered for the analysis of diffraction on non-periodic microscopic inhomogeneities and on periodic objects – subwavelength diffractive gratings. As examples, problems of diffraction of plane electromagnetic waves on dielectric and conductive cylinders with the diameter equal to the wavelength are solved. The finite element method is also used to solve the problem of diffraction of a plane wave on a one-dimensional binary dielectric grating with a period of fractions of the wavelength to several wavelengths. Another variation of the FEM is related to the solution of the integral equation of diffraction on a uniform sampling grid. In this case, the problem is reduced to solving a linear system of Gauss algebraic equations. In contrast to the boundary element method, this method does not require the calculation of derivatives of the field, normal to the boundary surface of the local inhomogeneity. A solution of the problem of diffraction of a plane wave on a multilayer dielectric cylinder in the form of a series of cylindrical functions is presented. The coefficients of the series in a general case are found from the recurrence relations. Explicit formulas for the coefficients of the series were derived for a two-layer cylinder. These methods were used to simulate the diffraction of light on Luneburg and Eaton–Lippmann gradient microlenses. This chapter also considers an iterative method for solving integral equations for electromagnetic diffraction of waves with the TE- and TM-polarizations. The conditions under which this method has a relaxation, i.e., is a reduction of the mean error with increasing number of iterations, are determined. The method effectively allows to calculate the diffraction field inside and outside the dielectric inhomogeneity of a size equal to or less than the wavelength.

The fourth chapter is a numerical method for solving the problem of diffraction on periodic diffractive micro- and nanostructures. The method is used to calculate and study the diffraction structures for a number of modern trends in nanophotonics, including plasmonics, metamaterials, nanometrology. The method of rigorous coupled-wave analysis (RCWA) is used to solve the problem of diffraction of a plane wave on two- and three-dimensional diffractive structures and diffractive gratings. This numerical method for solving Maxwell's equations is focused on the analysis of micro- and nanostructures described by a periodic function of the dielectric permittivity. Surface electromagnetic waves (SEW) (surface plasmon–polaritons) are studied, and calculation and study of diffractive structures designed to form interference patterns SEW are carried out. The diffractive structures are composed of a dielectric diffractive grating and a metallic layer deposited on the substrate. The parameters of the diffractive structure are calculated from the excitation conditions at the lower boundary of the metallic layer of a given set of surface electromagnetic waves of different configurations and directions. As a result, directly below the metallic layer there forms a periodic interference pattern of surface electromagnetic waves. Periods of generated interference patterns significantly subwavelength. A promising area of application of the considered structures is nanolithography based on registration of interference patterns of surface electromagnetic waves in the electron resist. The magneto-optical properties of bilayer metal–dielectric heterostructures consisting of a metallic diffractive grating and a dielectric magnetized layer are studied. The calculations show that these structures have resonant magneto-optical effects due to the rotation of the polarization plane of the incident wave and change of the reflectance (transmittance) index of the structure when the magnetization of the layer changes. These structure can be used as magnetic field sensors, gas sensors, light intensity modulation devices, controlled by the external magnetic field.

The fifth chapter describes the simulation of electromagnetic waves in nanophotonic devices. The FullWAVE software is used to calculate the passage of light through two-dimensional photonic crystals in the case in which the light frequency does not fall into the stop band. The results of modelling sharp focusing of light by the two-dimensional gradient photonic–crystal lenses, as well as the results of using these lenses as a coupling device for matching the two planar waveguides with different widths, are considered. It is shown that the width of the focal spot, which is formed near the surface of the photonic crystal (PC) lens, is equal to 0.3 wavelength. The results of experiments with fabrication of two-dimensional photonic-crystal lenses in a film of silicon on fused silica are outlined. The chapter also discussed the radial FDTD-method, which is adapted to solutions of Maxwell's equations for an axially symmetric diffraction laser beam with radial polarization on an axially symmetric optical element. The results of modelling of sharp focusing of laser light with radial polarization using a microaxicon and Mikaelian three-dimensional gradient lenses are

presented. The simulation results showed that in both cases focal spots are formed near the surface of the optical element with the inhomogeneous surface waves involved in their formation and it is therefore possible to overcome the diffraction limit. The diameter of the focal spot at half intensity was equal to 0.35 of the wavelength.

The sixth chapter discusses two methods of calculating the spatial modes of microstructured photonic crystal fibres (PCF). This is a relatively new class of optical fibres, which uses the properties of photonic crystals. In the cross section the PCFs have a quartz or glass microstructure with a periodic or aperiodic system of microinclusions, mostly cylindrical microperforations, oriented along the fibre axis. The 'defect' of the microstructure, corresponding to the absence of one or more elements in its centre, is the core of the optical fibre, providing a waveguide mode of propagation of electromagnetic radiation. Two methods for calculating the mode of optical fibres are discussed in detail: the approximate analytical method of matched sinusoidal modes, and grid method based on the use of finite-difference approximations to the stationary wave equations. The basic idea of the method of matched sinusoidal modes (MSM-method), also known as the transverse resonance technique, is based on dividing the PCF section into homogeneous rectangular areas, and the description in each field of a homogeneous area using a system of local sinusoidal modes. The MSM-method is modified by the iterative Krylov method in the most computationally complex stage of the solution of the non-linear problem of eigenvalues of the large matrix to which the problem of finding the propagation constants of modes is reduced. The MSM-method was used to calculate both scalar and vector modes of conventional round step-index fibres and the modes of photonic crystal fibres with a filled core. The basis of the finite-difference method (FD-method) under review in this chapter is the approach based on the use of finite-difference approximations to the stationary vector wave equations for monochromatic light such as the Helmholtz equations. The FD method wins in the speed of the algorithm in the MSM method because the problem of finding the propagation constant and the sampling grid solutions for the transverse components of the electric or magnetic components is directly reduced to a linear matrix problem for the eigenvalues and vectors. The FD method also allows for full vector analysis of modes of photonic crystal fibres with a hollow core. Examples of calculation of modes of Bragg fibres with filled and hollow cores are presented.

The seventh chapter contains the theory of paraxial and non-paraxial laser beams with axial symmetry and an orbital angular momentum. Such beams are called vortex beams, because their energy is propagating in a spiral around the optical axis, forming a 'funnel' as with a wind swirl. In nanophotonics the vortex laser beams are used for optical trapping and rotating micro- and nanoparticles in a ring in the cross-sectional plane

of the beam. In near-field diffraction the radius of the ring of the optical vortex is comparable with the wavelength, and considering this radius for the specified intensity level, the radius of the optical vortex can be several times smaller than the wavelength. This property of vortex laser beams is used in modulation nanolithography .

This chapter examines the diffraction of plane, Gaussian and conical waves on a spiral phase plate and a spiral axicon. Explicit analytical expressions are presented for the complex amplitudes of light of vortex beams in the area of Fresnel diffraction and far-field diffraction. The Rayleigh–Sommerfeld integral is used to study paraxial and non-paraxial vector theory of vortex laser beams. It is shown that for the beam waist radius close to the wavelength, the longitudinal component of the vector of the electric field is only a few percent of the transverse component. Considered are the scalar paraxial hypergeometric beams formed by the logarithmic axicon and spiral phase plate. The complex amplitude of the vortex laser beams is proportional to the confluent hypergeometric function or Kummer function. In addition, the family of such hypergeometric beams forms a basis, they all have a ring structure (the intensity on the optical axis is zero), and the thickness of the intensity rings of the transverse diffraction pattern decreases with increasing ring number, tending to zero in the limit. A special form of hypergeometric laser beams are hypergeometric modes that retain their intensity during propagation in space. Non-paraxial hypergeometric beams whose complex amplitude is proportional to the product of two Kummer functions are discussed. Numerical examples of the propagation of such beams and the experimental results on the formation of vortex laser beam using diffractive optical elements are presented.

The eighth chapter discusses methods for calculating the force and torque, exerted by the electromagnetic field focused onto the microparticle of arbitrary form, whose dimensions are comparable with the wavelength of light. There are two ways of calculation of light pressure on the micro-object: the rigorous electromagnetic method (two-dimensional case) and the geometrical optics method (three-dimensional case). The results of both methods of calculation of the pressure force of a Gaussian beam on a dielectric microcylinder are compared. The chapter also describes optical circuits, including diffractive optical elements (DOE) that form the laser vortex beams: Bessel mode, hypergeometric modes of different orders. Such DOEs are produced by optical and electron lithography. In some experiments vortex laser beams were formed by the dynamic liquid crystal microdisplays. The results of the experiments with multiorder optical elements forming multiple vortex beams having different angular orbital angular momentum are discussed. The diameters of the light rings on which microparticles rotated, were tens of microns, and the linear velocity of rotation was equal to a few microns per second.

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