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Optical field distribution in quasy-1D nanostructures

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Abstract. The FDTD optical distribution model in the quasi single dimensional nanostructures is presented. The polar diagram is analyzed for nanowire structure with various diameters. The main conditions for the maximum output in vertical (0° and 180°), horizontal (90°) and leaky mode (30° , 60° and 165°) directions are discussed. Theoretical data show good agreement with experiments.

1. Introduction

One dimensional (1-D) nanostructures such as nanowires (NW), nanotubes, nanobelts and nanosprings are fast becoming a key instrument in intensive research due to their unique potential for fabrication into high density optoelectronic nano-scale devices [1]. In fact, 1-D nanostructures are the smallest dimension systems that can be used for efficient transport of electrons and are thus critical to the function and integration. Their electrical properties are strongly influenced by minor perturbations due to high surface-to-volume ratio and tunable electron transport properties. Compared with the thin-film/thin-film LEDs [2-4], which may suffer from the total internal reflection, nanowire/thin-film heterostructures are utilized in order to increase the extraction efficiency of the LEDs by virtue of the waveguiding properties of the nanowires and decreasing the defect density of the carrier's nonradiative recombination [5-8]. Growth technique is developed to create the real optoelectronic devices based on nanowires [9-12]. Optical field distribution in such structures depends on geometrical and material parameters and can be easily analysed using numerical simulation. In this work, the structure is modelled using using finite-difference time-domain (FDTD) principle [13]. In this method, space is divided into small blocks representing the materials in the region of interest. Then by taking small steps in time, the propagation of the electromagnetic field is followed through space as it enters the region and interacts with the structure. The method allows for the effective and powerful simulation and analysis of sub-micron devices with very fine structural details. A sub-micron scale implies a high degree of light confinement and correspondingly, the large refractive index difference of the materials (mostly semiconductors) to be used in a typical device design. Some modal properties of circular section nanowires have already been described by Maslov and Ning [14-16] and others. These properties include the dispersion for guided modes, the end-facet reflectivity [14], the mode quality factor [17], the far-field emission [15], and the distribution of the emitted power between the free-space modes and the guided modes for an axial heterostructure configuration [16].

In this work we analyze angular optical field distribution in the single NW with different diameters.



2. Theoretical simulation

The finite-difference time-domain (FDTD) method for electromagnetic fields is a computational method for solving Maxwell's equations on a discrete grid in space and time [18]. With it, the real-valued time-dependent electric and magnetic field for a point in time and space are deduced from the surrounding electromagnetic fields a short time interval earlier. In this manner, the evolution of the fields can be followed. The concept of the FDTD method is thus very intuitive as it is closely related to how we experience the physical universe.

Solutions calculated with a basic FDTD method converge with second order with respect to the number of the grid cells per unit volume, but only if there are no material interfaces present. All simulations are performed as if the scatterers are contained in a perfectly conductive box. To obtain a unique solution to a given problem, in addition to the governing differential equations, boundary conditions have to be specified. An efficient implementation of an absorbing layer, called the perfectly matched layer (PML) is used in this calculation [19].

2.1. Model description

The model consists dot optical source inside single NW. A quantum dot can be modeled by a source dipole with in-plane orientation if we consider that the lateral confinement is not important (same behavior as an axial quantum well) [20]. NW is characterized by fixed normalized length ($L = 13\lambda/n$), optical source position ($h = 6.5\lambda/n$), period ($T = 4\lambda$) and variable diameter ($D = k\lambda/n$) where n is the refractive index, λ is wavelength and $k = 0.05-2$ is variable parameter (Figure 1).

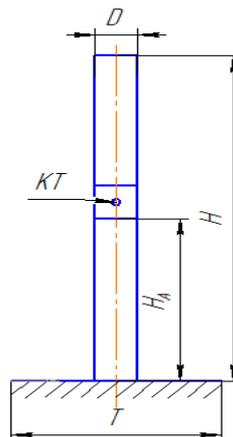


Figure 1. NW structure used in simulation

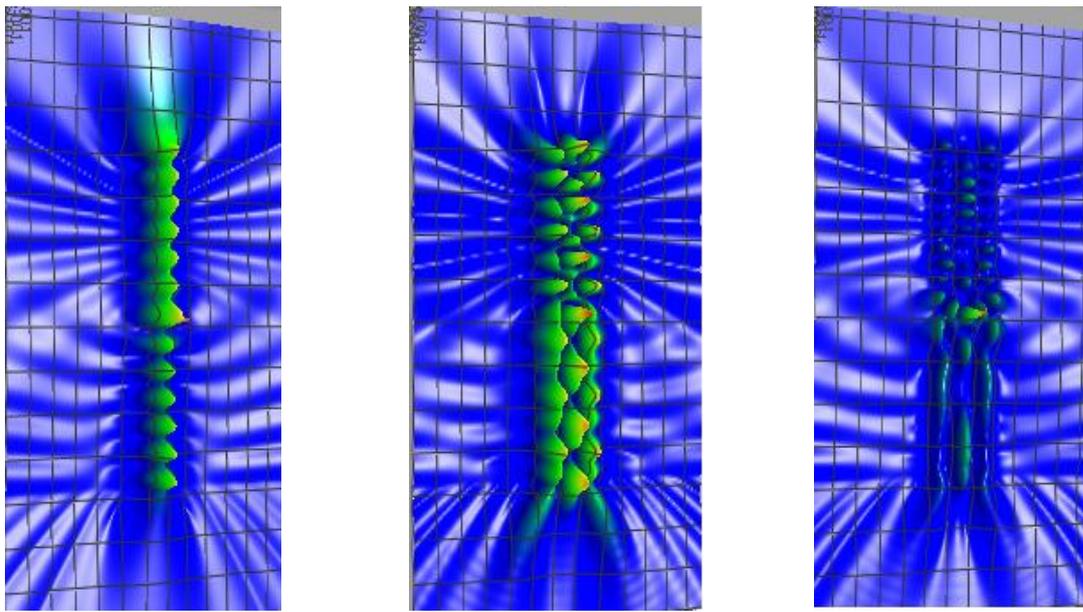
2.2. Optical field distribution in nanowire

Calculated results of E field distribution in the NW for different k are presented in Figure 2. Results show that perfect confinement of the optical field is possible for structure with k is less than quarter wave.

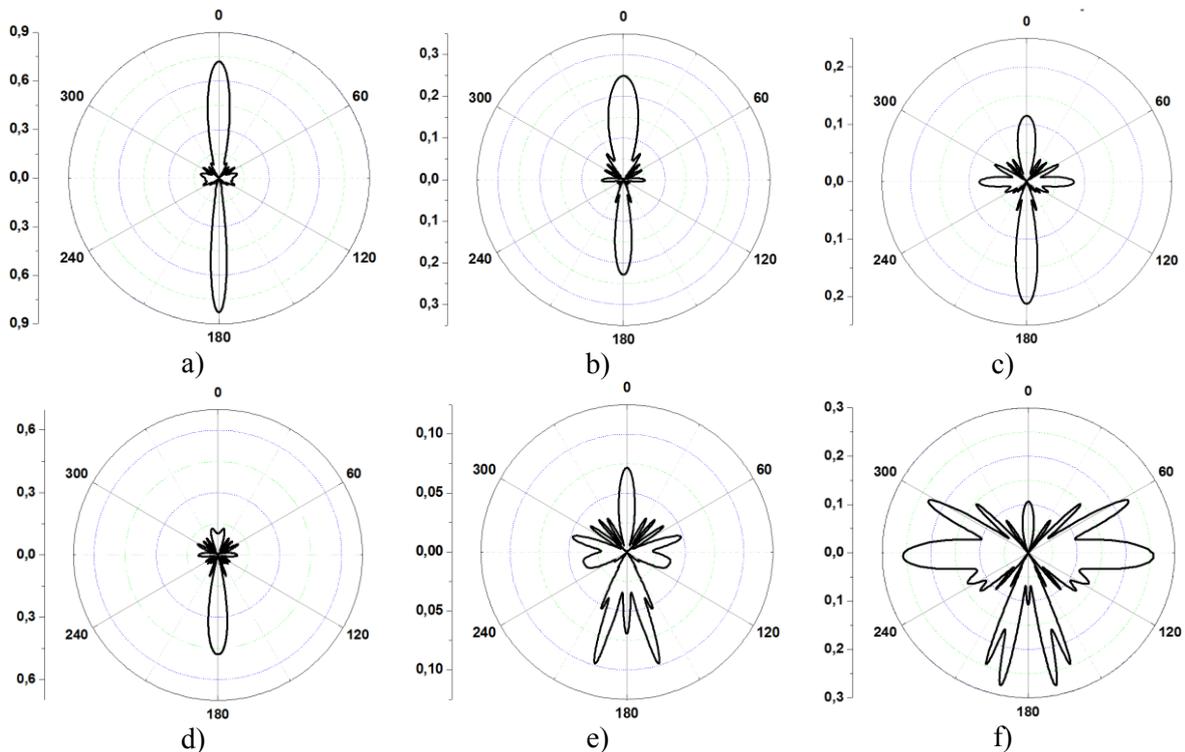
2.3. Polar diagrams and modes in the structure

Results presented on Figure 2 were transferred in the form of polar diagram for analysis of the NW optical properties for different normalized diameters ($D = k\lambda/n$) (Figure 3). Polar diagram shows five main directions of the light distribution: vertical (0° and 180°), horizontal (90°) and leaky mode (30° , 60° and 165°). For thin structures with k region 0.1-0.35 optical field transfers mostly in the vertical direction. Horizontal distribution prevails for NW with $k=1, 2, \dots$ that is in good agreement with interference law and measured PL intensity [21].

We also found that at $k=1.25$ and 1.6 strong and narrow leaky modes are transferred.



a) b) c)
Figure 2. E field distribution in nanowire for k equal a) 0.1; b) 1.25; c) 2



a) b) c) d) e) f)
Figure 3. Calculated polar diagrams for k equal a) 0.1 b) 0.35 c) 0.8 d) 1.2 e) 1.6 f) 2

Figure 4a shows dependence of the normalized diameter on the amplitude in each direction. For $k = 0.05-0.85$ light radiates mainly in vertical direction (up to 90%). The relation between up and down directions changes non-monotonically and quasi-periodically. At $k=1$ and 2 light distributes laterally that in agreement with field interference effect. At $k=1.25$ and 1.6 field redistributes in the leaky mode (30° , 60° and 165°) with narrow bandwidth. Calculated results agree well with different experimental data presented by plus markers (Figure 4b) [22-25].

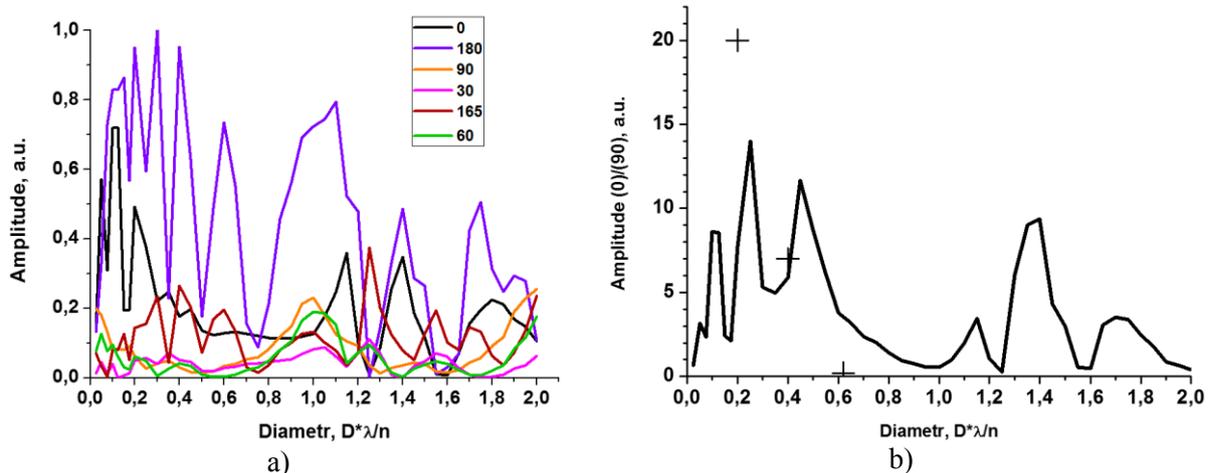


Figure 4. a) Calculated angular modes b) Vertical/horizontal mode amplitude relation vs diameter

3. Conclusions

In this paper we have investigated the optical properties of the near fields generated by a nanowire laser. The polar diagram of the light distribution in the linear nanostructures is analyzed for different structure diameters. For diameter lower than optical wavelength light mainly distributes in vertical directions. For structure with whole wavelength diameters light prevails in horizontal direction due to interference. We found conditions at $k=1.25$ and 1.6 with strong and narrow leaky modes.

Acknowledgments

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