様　式　Ｃ－１９、Ｆ－１９、Ｚ－１９　（共通）

科学研究費助成事業　　研究成果報告書

平成 ２７ 年　 ６ 月　 １ 日現在

機関番号： １２１０２
研究種目： 基盤研究(C)
研究期間： 2012～2014
課題番号： ２４５６００７１
研究課題名（和文） 囁きの回廊モード共鳴を用いたナノセンサーと信号処理素子のシミュレーションデザイン

研究課題名（英文） Simulation Design for Nano sensor and Signal Processing Devices based on Whispering Gallery Mode

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交付決定額（研究期間全体）：（直接経費）　4,200,000円

研究成果の概要（和文）：＊囁きの回廊モードを円筒、四角、三角などで試し、光学特性として円筒が最適であることを確認した。＊実部の銀のナノロッドアレー（直径10～20nm、間隔20～50 nm）に関して、誘電率の実部が負であり、可視光領域の場合の光学的特性の計算を行った。＊これらのプログラムはスパコン上で並列化を行った。＊ＦＤＴＤを使い逆解析によりイメージを再構成する方法も新規に発見した。＊離散的グリーン関数法に関する証明も行い、副産物として逆時間ＦＤＴＤにより形状を再構成する新たな方法を発見した。計算は膨大な量になり注意してアルゴリズム化しないと数値不安定となる。これらの問題点を克服し、良い結果を得た。

研究成果の概要（英文）：*We investigated WGM resonances for dielectrics of different shapes(such as cylindrical, elliptical, square, and triangular).We found that cylindrical resonators have the best optical properties for fabricating practical devices. *We computed the optical properties of different arrays of silver nanorods(10-20 nm in diameter, spacing 20-50 nm) in the visible wavelengths(400-700) nm, where the real part of the electrical permittivity is negative and the rods are thus effectively a metamaterial. We found that by adjusting the spacing and diameter linear arrays oriented perpendicular to the incident light beam (assumed to be Gaussian)the transmitted wavelength can be finely controlled with very low losses.*Some of them were implemented on a supercomputer.*We devised an optimization method to better represent curved boundaries on a rectangular grid .*We improved the calculation accuracy by using a new source model.*We have verified a discrete Green's function computational methodology.

研究分野： Nano-optical simulation and design using NS-FDTD

キーワード： silver nanorods　metamaterial　whispering gallery mode　recursive convolution　FDTD　time-reversed FDTD

1．研究開始当初の背景

(1) We have developed a new version of FDTD called nonstandard (NS) FDTD, for which the error is $\delta \sim (h/\lambda)^6$. NS-FDTD makes it possible to obtain high accuracy solutions of certain kinds of problems with a low value of λ/h. Because, the size, s, of the particles is small compared to the wavelength ($s = \lambda$), λ/h must be large in order to represent the particles on the numerical grid – even though the accuracy of the algorithm is high for a low value of λ/h. In addition NS-FDTD cannot be used to compute the optical properties of dispersive materials or when $\mathrm{Re}(\varepsilon)$ is negative.

The Whispering gallery modes (WGM：**囁きの回廊モード**) in a nanocylinder computed using NS-FDTD are shown in Fig. 1. This simulation used to consider dielectric sphere to be impossible using FDTD method because it takes very long time to excite Whispering gallery mode. However, thanks to high accuracy NS-FDTD method, Fig. 1 shows the first Whispering gallery simulation using FDTD in the world. We are confident using these sophisticated and high accuracy method inverse problem for Plasmonic devices can be solved.

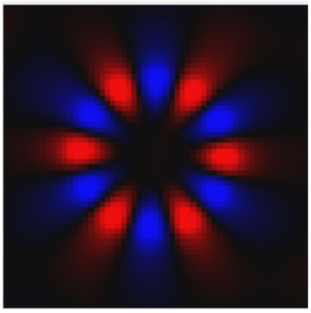

Figure 1． Whispering gallery modes in a dielectric nanocylinder computed using NS-FDTD . Wavelength = 700nm, diameter = 350nm, refractive index = 2.72. Resonances are very sensitive to the details of the algorithm.

(2) Optical Whispering Gallery Mode Resonators in the Mie Regime

In what is called the Mie regime, the size of particle is about equal to the wavelength of the light, with which it interacts. For visible light the Mie regime is about 100–2000 nm, and for near infrared, used in optical communication, it is about 200–2000 nm.

Acoustical whispering gallery modes are often observed in domes of churches and halls, where sound waves interfere in such a way that the sound very loud in some places, but is nearly zero in others. An optical whispering gallery modes can be observed in solid dielectric cylinders and spheres. Fig. 2(a) shows a typical example. A light source (yellow) is embedded in a dielectric (blue). For a refractive index of and radius = 0.5 wavelength, the pattern of light intensity (shades of red) is seen in Fig. 2(b).

Whispering Gallery Mode Sensors: refractive index, stress and strain, contaminants

In the Mie regime, where the wavelength is about equal to the size of the resonator, the modes are very sensitive to small changes in both the refractive index and shape.

Fig. 2(b,c) shows how intensity pattern of the light leaving the resonator changes for small change in the index of refraction (n). Changing the shape by a small amount also changes the light intensity pattern, for example squeezing the height but keeping the width constant.

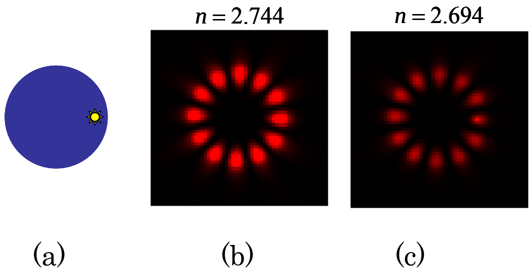

Figure 2. Mie regime whispering gallery mode resonator. (a) Source (yellow) embedded in dielectric material (yellow). (b, c) Intensity (shades of red) of optical modes for different refractive index.

Changing the refractive index or the shape by just 1% produces a detectable change in the light pattern. If a particle touches the resonator, the output light pattern also changes. Thus using WGM resonators in the Mie regime it is possible to make small sensors that detect changes in pressure, stress, strain, and refractive index, and which can detect the presence of nanometer–size biological and chemical particles. The sizes of these sensors are only a few hundreds of nanometers.

Because of their small size thousands of such sensors could be place on a silicon chip of a few square millimeters.

２．研究の目的

We design a prototype for an intelligent optical biosensor system based on an array of coupled whispering gallery mode resonators in the Mie regime linked to an artificial neural network. We train this network to recognize biological materials by their optical properties – from the way they perturb the array system..

３．研究の方法

(1) Model Development

Many possible array configurations (for example triangular or square array) are possible, and whispering gallery mode resonator designs. By adjusting the size and refractive index the resonance frequency can be selected. For our purposes a wavelength of about 500 nm is suitable, but we would like to adjust it slightly to optimize detection of different biomaterials. This can only be done by numerous simulations. In particular we need study the effect of orientation on signal strength for rod-shaped bacteria.

(2) Implementation and debugging of computer programs

We already have template programs, but they need to optimized and speeded up. The design problem is essentially an inverse problem, so simulation speed and effective use of memory is essential. We have already set up MPI (message passing interface) and Open MP for shared memory. With Dr. S. Banerjee, Sumitomo Kagaku.

(3 Design calculations

We have narrowed down the choices two basic array types: square – which so far seems the most promising – and triangular. Simulations with test particles of different types will be done the goal is

- Maximize the number of bacteria (different sizes, shapes, refractive indices) that can be detected,
- Maximize signal strength.

４．研究成果

(1) We have developed high-accuracy finite-difference time-domain (FDTD) algorithms, that deliver high accuracy on a coarse space-time grid. However when dealing with a resonant structure, such as a whispering gallery mode resonator, the accuracy is limited

not by the FDTD algorithm, but by the representation of the structures on the spatial grid.

Off resonance, it is possible to use what is called the “fuzzy method” in which values of the material parameters (index of refraction or electrical permittivity) in between the grid points are used to adjust the values of the values at the grid points – see Fig.3.

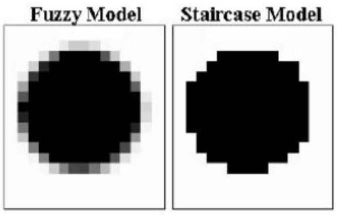

Figure 3.

However on resonance, this method is not accurate enough. One would like to have a broad-band adjustment that works for all frequencies, but unfortunately this is impossible. But within a limited frequency band (for example $\pm$ 10% of the central frequency) using the Mie theory of layered spheres and cylinders, we can adjust the material parameters at the grid points.

Fig. 4 shows a one-dimensional example. We wish to represent a layer of width w and refractive index n_s, on a grid where $x = \chi\Delta x$ where $\chi = 0,1,2,\cdots$ is an integer but $w/\Delta x \neq$ integer. We can represent this single layer by two outer layers of width Δx and refractive index n_b, and a central layer of width $m\Delta x$ and refractive index n_a , where m is an integer. We can fit the values of n_a, n_b and m so that the transmission and reflection spectrum of the three-layered structure matches that of the original one-layer on a given frequency band.

This is more accurate than the fuzzy method. In a similar manner (even for objects that are not spheres or cylinders we can get better accuracy than the fuzzy method).

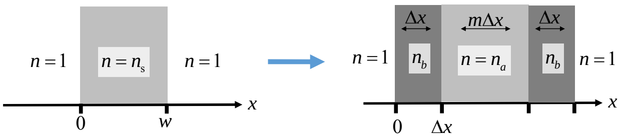

Figure 4

These results were presented at ACES (Applied Computational Electromagnetics Society) Conference in 2015.

(2) Optical whispering gallery mode resonators in the Mie regime (size on the order of a wavelength) are extremely sensitive to small perturbations and to changes in their environment.

For example, a dielectric disk of diameter = 1500nm and refractive index $n = 2.74475$, has a whispering gallery mode (WGM) resonance at wavelength = 1500nm in the TM mode (electric field parallel to the disk axis).

We performed calculations using our new high accuracy algorithm finite difference time domain (FDTD) algorithm based on a nonstandard finite model, and found that a shift in the refractive index of $\Delta n/n = \pm 1\%$ reduces the resonance intensity by about 63% . Such a shift could be induced by heating, strong illumination, or by adsorption of foreign substances such as proteins and bacteria.

Small perturbations in the external environment also affect the on the resonance. According to our calculations, a particle of diameter = 750nm and refractive index = 1.4 (roughly typical of bacteria and proteins,) touching the WGM resonator causes the resonance intensity to decrease by about 40%, and up to an edge to edge separation of 750 nm away the decrease is some 10%, which can easy be detected.

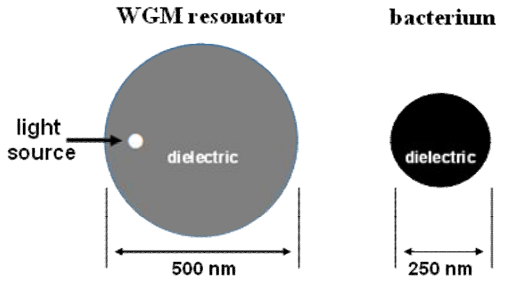

Figure 5 A whispering gallery mode is excited by a light source. The light intensity inside and outside the resonator is affected by the presence of a bacterium (modeled as a particle 250 nm in diameter of refractive index =1.4).

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〔その他〕
ホームページ等

http://www.cavelab.cs.tsukuba.ac.jp/nsfdtd/jp/

６．研究組織

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