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Simulation and optimization of multilayer-coated microsphere in temperature and refractive index sensing



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ABSTRACT

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1. Introduction

Microsphere resonators supporting optical whispering-gallery modes (WGMs) have been extensively studied over the past decade in many fields including narrow linewidth microlasers [1], nonlinear optics [2], and miniature sensors [3–8]. Due to the advantages of high quality factors (Q) and low mode volumes [9], microspheres are widely used as high sensitivity temperature and RI sensors, which usually employ the measurement of wavelength shifts of WGM resonance resulting from the change of effective refractive index and/or size of the resonator. For instance, Dong et al. demonstrated experimentally a highly sensitive temperature sensor based on the polydimethylsiloxane (PDMS) microsphere with the resolution of 2×10^{-4} °C [3] and Hanumegowda et al. realized a microsphere RI sensor with a detection limit 10⁻⁷ refractive index unit (RIU) [6]. Moreover, Vollmer et al. developed a WGM microsphere resonator biosensor which achieved label-free detection down to single molecules [7].

Although the microsphere resonator sensors own very high sensitivity, they also bring about some defects. As we know, the resonance wavelengths are susceptible to thermal fluctuations due to the probe-induced energy absorptions and environment temperature changes. Decreasing the input laser power to the resonator can reduce the optical absorption, however, the environment temperature is not controlled in some occasions. To compensate the thermal drift, the most common method is coating the microresonator with materials of negative thermo-optic

This study proposes an approach to simultaneously detect the refractive-index (RI) and temperature changes with a three-layer-coated microsphere resonator. The RIs of the three layers are high, low, and high from inside to outside. Using the perturbation theory and finite element method (FEM), a model is developed to calculate the RI and temperature sensitivities for the inner mode and outer mode, respectively. As a result, a second-order sensing matrix is defined to determine the RI and temperature changes. By optimizing the coatings thickness, the thermal noise can be eliminated with the differential frequency of outer and inner modes.

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coefficient [10], which is proposed by Han et al. Moreover, He et al. have experimentally demonstrated the feasibility of this method by applying a thin layer of polydimethylsiloxane (PDMS) to the surface of the silica resonator [11]. It should be noted that a precise control of the coated layer thickness is required to eliminate the thermal drift, which is difficult in practice. Besides, Le et al. experimentally investigated a novel method to reduce the thermal noise without modifying the conventional coupling system, which exploits the different sensing properties between transverse magnetic (TM) modes and transverse electric (TE) modes [12]. However, the common disadvantage of these methods is that the sensors cannot detect the temperature and RI simultaneously.

In recent years, self-reference concept based on multilayer films has been successfully applied in the resonant mirror device for dispersion compensation [13] and surface plasmon resonance (SPR) structure for background-free detection [14] in sensing fields. Obviously, it can also be used in WGM microresonator. In this paper, we investigate the three-layer-coated microsphere and propose that this new-style structure can be used as a sensor which not only reduces the thermal effect in RI sensing but also detects temperature change simultaneously. The sensor concept and its working principle are illustrated in Section 2. In Section 3, the theoretical model to calculate the resonant wavelength shift due to the variations of surrounding medium RI and environment temperature is developed based on the perturbation theory proposed by Teraoka and Arnold [15]. In Section 4, the WGMs in the triple-coated sphere and the influence of the middle layer thickness on the RI sensing property are investigated in detail. Furthermore, we calculate the thermal induced shift of the resonance wavelengths for the inner and outer modes and conclude that the

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thermal effect can be eliminated by the optimization of the outer layer thickness. At last, some meaningful results are summarized in Section 5.

2. Sensor concept

This paper proposes a versatile WGM-based sensor by applying three layers to the surface of a plain silica microsphere as shown in Fig. 1. The RIs of three layers are high, low, and high in turn from inside to outside. A tapered fiber is positioned close to the coated microsphere to couple the incident laser. The diameter and RI of the tapered fiber should be appropriate to excite the desired WGMs in the high-RI layers [16]. An optimal gap between the coated sphere and tapered fiber is necessary to guarantee the performance of the sensor. As discussed in Ref. [17], each of the two high-RI layers (A and C) can support its own WGM, which is called inner mode and outer mode, respectively, if the middle layer RI is sufficiently low and its thickness is appropriate. The resonant wavelengths of the two modes split, just like the coupling of the WGM in two spheres. Thus, when the propagation constant of the mode in the fiber matches with that of the WGM in the coated sphere, the light couples into the high-RI layers and results in spectral dips in the transmission spectrum.

The sensor detects the changes of the environment temperature and RI by simultaneously monitoring the resonant wavelength shifts ($\delta \lambda_{R,i}$ and $\delta \lambda_{R,o}$ in Fig. 1) of the inner and outer modes. These two modes have nearly identical changes with the temperature variation yet significant differences in sensitivity to the RI change of the surrounding. Thus, we can use the differential wavelengths of inner and outer modes to reduce the thermal noise in a certain extent in RI sensing. Accurately, we can define a secondorder sensing matrix to obtain the RI and temperature changes simultaneously. Compared with the traditional monolayer-coated microcavity sensors which can eliminate thermal noise [10,11], the



Fig. 1. The configuration and sensing principle of the versatile sensor based on three-layer-coated microsphere. The sphere is shown in spherical polar coordinates (r, θ , and φ), n_0 , n_A , n_B , n_c and n_1 are the refractive indices of the surrounding medium, layer A, B, C, and the microsphere, respectively. $\delta \lambda_{io}$ is the spacing between two adjacent resonant dips in transmission spectrum. $\delta \lambda_{R,i}$ and $\delta \lambda_{R,o}$ represent the resonant wavelength shifts of the inner mode and the outer mode, respectively, due to the environment change.

three-layer-coated sphere sensor has three advantages: (i) the coating material can be selected more flexibly without restriction on the thermal-optic coefficient; (ii) the coating can be deposited by RF magnetron sputtering which is different from PMMA and PDMS and the thickness can be precisely controlled; (iii) the sensor is capable to detect the changes of environment temperature and RI simultaneously.

The main performance factors of the triple-coated microsphere sensor are detection sensitivity, detection limit, and detection range. These factors are related to a number of parameters including microsphere size, thickness and RIs of the three layers, radius of tapered fiber and its distance to the microsphere, and so on. The influence factors of detection sensitivity vary with different physical quantities to be detected. In thermal sensing, sensitivity is related to the thermo-optic coefficients and thermal expansions of the coating materials. However, in RI sensing, sensitivity depends on the percentage of the evanescent tail extending into the surrounding medium. The detection limits of RI and temperature changes are determined by the wavelength resolution $(\delta \lambda_R)_{min}$ which is affected by the WGM resonance linewidth and temperature fluctuation [18]. The detection range, determined by the difference $(\delta \lambda_{io})$ between two neighboring resonant dips in the transmission spectrum, is different from the free spectrum range FSR of the plain microsphere. For the triple-coated microsphere, the inner and outer modes have their own resonant spectrum and FSR (FSR_i and FSR_o as shown in Fig. 1), and the transmission spectrum contains both the inner and outer modes. As we know, the FSR is inversely proportional to the size of the resonator [19], leading to a larger FSR for the inner mode than the outer. Therefore, $\delta \lambda_{io}$ varies with different orders of the WGM and the maximum can reach up to $(FSR_i + FSR_o)/2$. A small $\delta \lambda_{io}$ will reduce the dynamic range of the temperature and RI measurement because of the difficulty to identify the corresponding order of the resonance dips. Obviously, as the same to FSR, $\delta \lambda_{i0}$ is related to the microsphere size. A large sphere results in a small $\delta \lambda_{io}$ but a high Q factor which can enhance the detection limit.

3. Theory and simulation model

3.1. WGMs in a triple-coated microsphere

In the past years, the WGMs and resonance spectrum of the microsphere resonators have been widely studied [20,21]. Arnold et al. theoretically analyzed the properties of different coated microspheres and calculated the field distribution of a WGM in a three-layer-coated microsphere [17]. Each WGM is characterized by three indices: l, m, and v, which represent angular, azimuthal, and radial mode numbers, respectively. We only concern the fundamental mode which is defined by v = 1 and m = l. Besides, the WGMs can accommodate two polarizations modes: TE modes and TM modes with the electric and magnetic fields parallel to the surface of the microsphere, respectively. Depending on the polarization of the coupling light in the tapered fiber, these two modes can be selectively excited with a polarization controller. In general, for TE and TM modes, there is a little difference between their responses to the RI and temperature variations. However, their properties and change tendencies are same, thus, for simplicity and without loss of generality, this paper considers TE modes only.

To our knowledge, the field distribution of the WGM and the resonance spectrum are determined by the geometry and spatial distribution of the RI inside and outside the microresonator. We consider a plain microsphere with refractive index of n_1 , coated by three layers with thickness of t_A , t_B , and t_C , and RIs of n_A , n_B , and n_C as shown in Fig. 1. It should be noted that the high-RI layers are the same materials ($n_A = n_C$), and the materials of middle layer B

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