Calibrated Fiber Grating Wavelength Combs Enable High Accuracy Biosensing

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Abstract: Simulation-based calibrations of measured spectra are used to find the exact optical properties of multi-resonant fiber gratings, resulting in elimination of cross-sensitivities, lower noise and orders of magnitude improvements in biochemical sensor limits of detection.

1. One fiber grating, many uses

A Tilted Fiber Bragg Grating (TFBG) in a single-mode fiber is really a shared grating embedded into two coaxial, co-located, very high-quality waveguides; one of which is single-mode (the core), and the other highly multimode (the cladding) with a V number larger than 250 [1-2]. The combined structure has hundreds of modes with highly different responses to various perturbations (Fig. 1). In particular, the core mode is only sensitive to axial strain and temperature, while cladding guided modes also "react" to bending, shear strains, and any change in the permittivity of the medium adjacent to the fiber surface [3-7]. Furthermore, each mode sensitivity to a given perturbation depends on its EM field distribution in the cross-sectional plane, on the polarization of the fields in the core and at the cladding boundary, and on the penetration depth and polarization of its evanescent field [2,8]. An obvious well-known example is that the refractive index sensitivity of cladding modes increases as their effective index decreases towards that of the external medium when they approach cutoff.

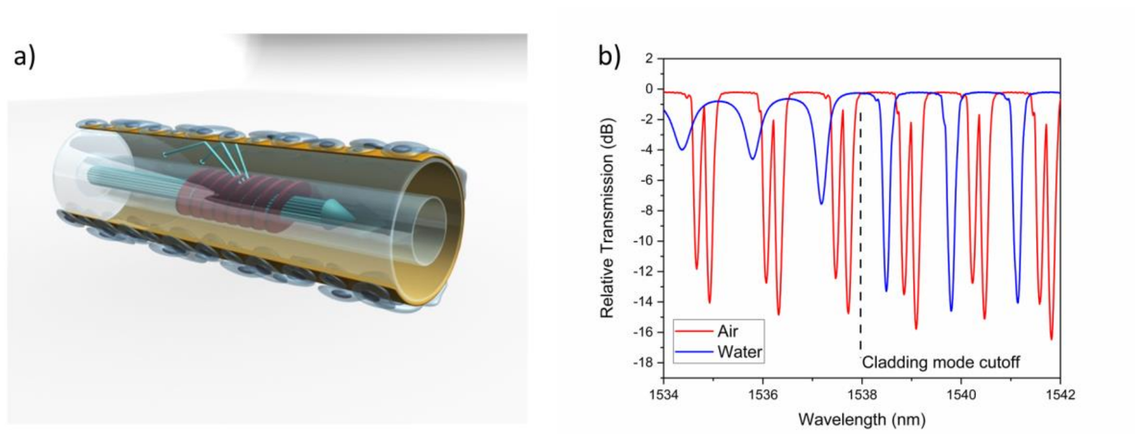

Fig. 1 a) Artist impression of a tilted grating in single mode fiber with cells attached to its surface; b) TFBG measured transmission spectra near cut-off in water and in air. Vector mode splitting is clearly observed in the "air" spectrum. Dashed line indicates cut-off in water.

This technology has been used extensively over the last 10 years or so in many sensing applications that include measuring temperature-independent strain, determining 3D shapes, performing absolute refractometry, quantifying protein binding, identifying molecules in food samples, monitoring ultrathin film deposition, probing live cell cultures, and detecting charge in supercapacitors [9-15].

2. Taking advantage of the vast amount of data in a TFBG spectrum

In most applications noted above, the sensing mechanism relies on using the core mode resonance to remove the impact of the local temperature on the quantity to be measured, and then following the wavelength or amplitude changes of a single resonance in the remainder of the spectrum, determined to be the "most sensitive" for the given application. For instance, this most sensitive resonance is often the last guided resonance before cut-off for evanescent field sensing, but a different one for bending and surface plasmon assisted sensing. While this approach has reached very competitive limits of detection, down to 8 nM for low molecular weight molecules in real food samples for instance [13], or 10 ppb for dynamic refractive index changes in air [15], it seems obvious that there is much more data to analyze in the complex TFBG spectra. The next level of improvement uses more than one of the cladding mode resonances, in addition to the core mode resonance to extract sensing information from relative shifts in the cladding mode spectrum, such as those shown in Fig. 2. In both cases, relative measurements can be used to remove "common mode" noise and systematic errors and thus improve detection limits and sensing accuracy.

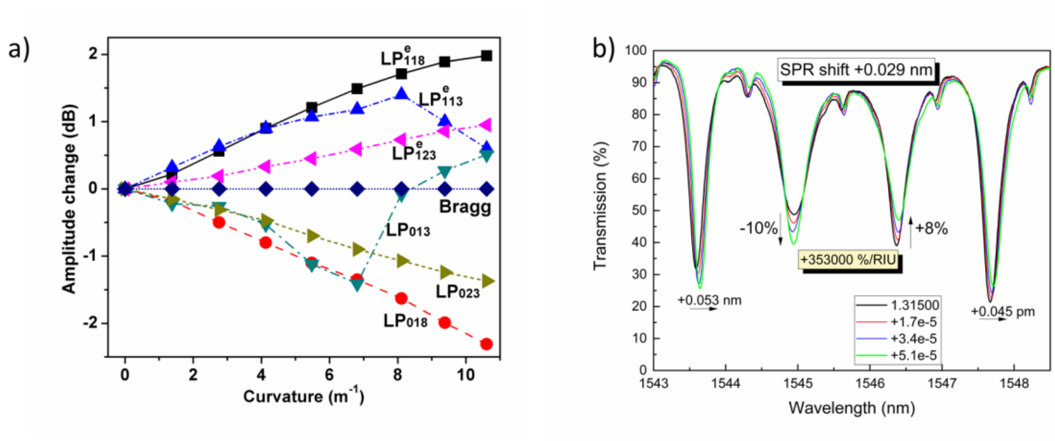

Fig. 2. a) Example of individual mode resonance amplitude shifts upon bending (from [4]); b) Example of mode resonance amplitude and wavelength shifts near the surface plasmon resonance in a gold-coated TFBG when the surrounding refractive index changes from 1.315 (water) by values indicated in the legend (from [16]).

2. Get to know your fabricated TFBG: creating a "perfect model" of a multi-resonant grating

In all applications of TFBG for sensing, ALL resonances move, and they move differently [17]. Therefore, if the response of many individual resonances to well-defined perturbations was known, then the shifts of many resonances could be "averaged" to extract the desired information. This averaging process would improve the measurement standard deviation by reducing noise on individual wavelength shifts and hence the detection limits. In order to do this, it is necessary to be able to predict very accurately the effect of material parameter or dimension changes (of the fiber, and of coatings and other surrounding materials) on the guided modes of the core and cladding. It turns out however that when using well-accepted single-mode fiber parameters in numerical models for Maxwell's equations are used to simulate TFBG spectra [18], the resonance locations are very different from those of corresponding measured devices (Fig. 3a).

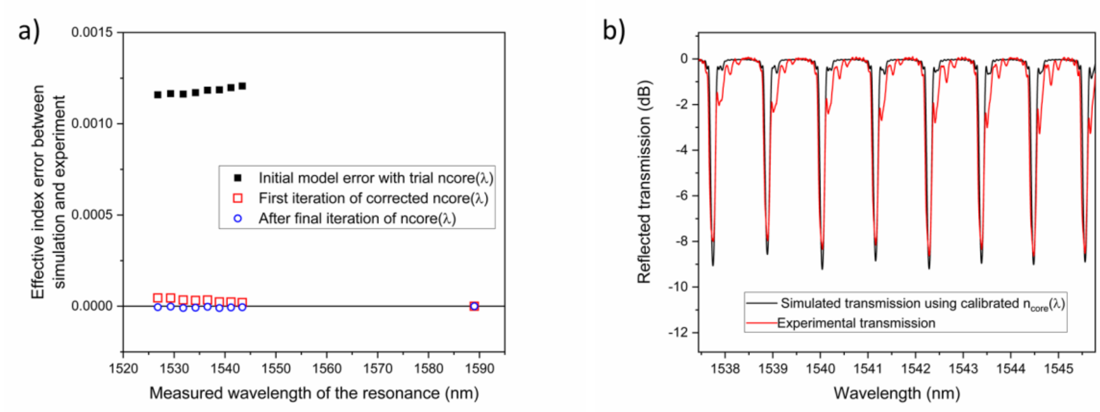

Fig. 3. a) Evolution of the error in effective index between the simulated and experimental resonance positions during the multistep calibration process; b) Comparison between the final simulation with the best value of the core index dispersion and the experimental spectrum.

This is because the grating inscription process increases the refractive index of the core (by around 0.001), and also its dispersion (by more than 50%) [19]. So, to model a real (fabricated) TFBG, the resonance positions of a measured spectrum in a strain free state and in air (the TFBG senses itself!) are used to find the new core index and dispersion values by an iterative process of successive improvements involving the minimization of the errors between simulated resonances relative to the experimental ones (Fig. 3b). In most cases the standard deviation of wavelength differences between measurement and simulation falls to 1 pm or less. Since in general only a few (3 to 5 at most) parameters are to be determined in sensing situations, having dozens of individual measurements from a single TFBG in a single experiment represents a largely over-determined mathematical inverse problem (and therefore solvable using the calibrated initial spectrum as a starting point), allowing measurements of parameter changes (such as surrounding index, absorption, or the complex refractive index and thicknesses of coatings) with accuracies of 1 part per million. It is worth noting that polarized spectra further allow the determination of indices of birefringent materials by probing separately with radially or tangentially polarized cladding modes [8,11,19].

In summary, the use of calibrated spectral combs of cladding mode resonances is proposed to develop multifunctional sensing systems using overdetermined inverse methods to link simultaneously a few measurands to the averaged spectral shifts of much larger numbers of individual cladding mode effective indices, thereby reducing the standard deviations relatively to measurements from single or few resonances. Basically, a single TFBG spectrum provides many "independent" measurements of the unknown parameters, with a device that has extremely low insertion loss and is compatible with widely available telecommunication instrumentation. These features make it competitive (in cost and performance) with most sensing technologies, not only fiber-based ones.

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5. References

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