Thermal Behavior of Waveguide Gratings

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ABSTRACT

We investigate the design of binary grating structures, e.g. resonance waveguide filters (RWFs), with subwavelength feature sizes, taking the temperature dependence of different material parameters into account. Our final goal is to demonstrate devices with athermal operation. We design the binary grating structures to be made in polymer substrates, such as polycarbonate (PC), due to their potential for low cost, mass fabrication. The high thermal expansion coefficient (TEC) of polymers, compared to inorganic optical materials, enhances the thermal sensitivity of the grating structures. The gratings are designed using Fourier Model Method (FMM) by considering both thermal expansion and thermo-optic effects on the resonance wavelength shift. The fabrication of RWF structures is proposed by e-beam lithography, creating a master stamp and copying the structures into a polymer substrate by some replication techniques, followed by an ALD deposition of TiO2. When the resonance waveguide grating RWG is designed for nearly room temperature operation at a peak wavelength of 633 nm with a full width half maximum FWHM of 3 nm (TM mode reflectance), the peak wavelength shifts 0.2 nm /5°C when only the TEC is taken into account. However, taking into account also the thermo-optic coefficients TOCs of PC and TiO2, the peak position shifts to 0.4 nm/ 5°C on the opposite side of spectral central wavelength. Thus the overall shift reduces to 0.2 nm /5°C, illustrating partial athermalization. It was also observed that thermo-optic coefficient TOC contributed more significantly than TEC effect. The wavelengths shift was almost linear with respect to temperature for both effects and showed slopes of 0.0673, 0.0422 and 0.02352 for TOC, TEC and combined effects, respectively.

Keywords: Diffractive optical elements, resonance waveguide filters, thermal expansion coefficient, thermo-optic coefficient.

1. Introduction

Diffractive optics has emerged as challenging micro optical structures since the recognition of the benefits of wave optical engineering over geometrical optics. Diffractive optical elements DOE of subwavelength dimensions are employed in a wide range of applications1,2. A diffraction grating is a spatially periodic modulation of refractive index that affects the amplitude, phase, or the state of polarization of an incident electromagnetic wave. This periodic refractive index modulation can be realized as a scattering structure in DOEs, which creates optically effective interface with respect to, for example surrounding material (air). DOEs can show guided mode resonance phenomena for incident electromagnetic waves over a selectable parameter range for device applications3. A selectable narrow reflectance
spectrum is obtained by coupling of the externally propagating modes with waveguide grating modes\(^4\). The grating modes coupling with the incident light can be calculated by solving an eigenvalue equation for the modes inside the modulated region. In addition, the resonances of evanescent waves couple strongly to diffracted waves which then results in a redistribution of total energy in propagating diffracted waves\(^5\).

In polymeric materials most economical, efficient and rapid replicated subwavelength structures of diffraction gratings are generated by standard high pressure heating tool techniques such as injection molding and hot embossing. Hot embossing is a two-step compression molding cycle in which already formed thin polymer film is heated through heat conduction near its transition temperature and then filling of the microcavities by compression in second step\(^6\). Amorphous TiO\(_2\) deposited by atomic layer deposition (ALD) is a high refractive index material and almost transparent across the entire visible range\(^7\). ALD is a modified form of chemical vapor deposition CVD, in which the film grows by means of a cyclic process through a series of surface reactions between the adsorbing precursor species and already left over reactive precursor species by previous pulse\(^8\). Thin TiO\(_2\) films deposited by ALD distinguish it from other deposition techniques in terms of atomic level thickness, composition, large area uniformity, thermal decomposition and film conformity control. A study shows waveguide properties of amorphous TiO\(_2\) films grown by ALD technique as resonant waveguide grating structures (RWGS) on glass and silicon which couple externally propagated light into a waveguide mode\(^9\).

In this paper we investigate the effect of various geometrical parameters on the thermal properties of guided mode resonance filters in polymer waveguide gratings. Since polymer materials are sensitive to thermal changes and results in variations of optically coupled field due to change in geometrical parameters of the grating such as interfacial profile, grating period, and fill factor. Two major factors contributing towards the shift of the center wavelength are, generally, thermal expansion coefficient and thermo optic coefficient of the polymer and dielectric materials\(^10\). A study illustrates the effect of high thermal expansion of polymeric materials to thermal sensitivity of center wavelength shift\(^11\). Various optical materials show increase in refractive index with respect to temperature that is they possess positive thermo-optic coefficient $dn/dT$, however, some optical materials and polymers show negative thermo-optic coefficients. The materials showing negative values of $dn/dT$ can be investigated for athermal optical device applications. Polymer materials such as polycarbonate\(^12\) and thin films of dielectric\(^13\) materials like TiO\(_2\) have negative thermo-optic coefficients and thus can be used in almost and/or partially thermally stable devices.

### 2. Diffraction Grating Optical Design

A diffraction grating illuminated by a directional wave generates a discrete set of diffraction orders. A simple binary, unslanted and planar grating structure in asymmetric waveguide geometry is designed in Polycarbonate PC material surrounded by air as shown in Fig. 1a. The PC grating is then coated by TiO\(_2\) layer by ALD deposition process as shown in Fig 1b. The designed grating period $d$ is 368 nm, fill-factor $0.38$, structure depth $h$ is 222 nm and TiO\(_2\) deposited surface layer thickness $t$ by ALD is 39 nm. When electromagnetic light incident on the grating at an angle $\theta_i$ ($8^\circ$) with the normal to the grating, reflected diffraction orders generate at the design wavelength, however, we considered only the zeroth order diffracted waves. The refractive indices of three regions are 1, 1.58, and 2.3401 for air, PC, and TiO\(_2\) respectively at wavelength 633 nm.

A rigorous analysis is required to compute the diffraction efficiencies of all diffracted orders which demands exact solutions of Maxwell’s equations and boundary conditions. We used in house written Fourier Modal Method FMM which is a versatile and stable rigorous analysis approach.

As far as we are concerned to the fabrication of real structures, the most significant designed geometric parameter is the aspect ratio in the polycarbonate material which depends on the line-width and the depth of the structure. The replication of grating patterns form master stamp to polycarbonate film can be obtained up to a certain aspect ratio after which exact grating lines are difficult to achieve. In addition, it is also challenging to fabricate structures with depth profile at a high
accuracy in master stamp. If a small error in depth profile is generated during dry etching of master stamp, the same would then be replicated with additional variations in PC. Furthermore, the edge profile of the structure in master stamp may have some variations at the top and bottom of a groove. The variations in depth profile of the replicated structure in PC can be tolerated and controlled by the ALD coating thickness. In Fig. 2a ridge height (pattern depth) is shown as a function of TiO$_2$ thickness. Since ALD films are much precise in thickness due to atomic level deposition and also known to perform as an independent process with respect to structure fabrication by e-beam lithography subsequent by dry etching and finally nanoimprint lithography NIL (replication). Fig. 2b shows variation in incident beam angle and reflected central wavelength with respect to rest of the other fixed geometrical parameters of structure. It shows that a particular reflected wavelength can be selected at a fixed incident angle and temperature, which can be applied in applications where Bragg’s reflectors are used. If however, temperature varies then central wavelength changes and one can find a relation between temperature and input angle. Thus, in this way by varying the input angle corresponding temperature changes can be calculated with respect to wavelength. Fig. 2c shows tolerance values of refractive indices of TiO$_2$ and PC over all other fixed parameters. Similarly, Fig 2d shows variation between fill factor and ridge height.

3. Results and discussion

The calculated reflectance spectra (TM Mode reflectance) at peak wavelength 633 nm with a full width half maximum FWHM of 3 nm at room temperature operation for the designed geometric parameters of structure is shown in Fig. 3a.

The position of the central wavelength was observed to shift towards longer wavelengths when temperature of (RWF) increases above the room temperature. Taking into account the contribution of thermal expansion coefficient TEC only of PC material ($7.02 \times 10^{-5}$/K) which leads to an increase in the periodicity of the structure and hence a corresponding shift in wavelength 0.2 nm/5°C towards longer wavelength as shown in Fig. 3b. However, taking into account also the TOC of TiO$_2$ and PC materials only, the central peak position of the TM mode reflectance shifted towards shorter wavelength 0.4 nm/5°C as shown in Fig 3c. It is evident from Fig. 3b and 3c that both effects result to a reverse change in the central wavelength, although not equal exactly. After combining both the effects we found the central wavelength position was partially stabilized at 5°C as shown in Fig 3d and thus illustrating partial athermalization. Theoretical studies show the same effect at higher temperatures but due to non linear changes of dn/dT an exact athermalization phenomena was absent. Since it is already reported$^{14}$ that the change in refractive index of TiO$_2$ shows linear relationship with density, on the other hand dn/dT changes are not exactly linear which may be attributed due to some environmental effects, however, it can be approximated as linear. The shift in wavelength position was studied up to a temperature change of 100 °C by considering the individual TEC, TOC, and the combined effects. The wavelength shift at various
temperatures are calculated and then plotted with respective temperatures to observe the effects of TEC and TOE. It was observed that both effects show almost linear variation with temperature and the effect of TOC is most significant compared to TEC as evident from Fig. 4. The individual effects are shown in Fig 4a and 4b with respective slopes of 0.0422 and 0.0673 for TEC and TOC respectively. The combined result is shown in Fig 4d showing a characteristic slope of 0.02352 which is less than the either individual effects demonstrate the partially athermalization operation of the structure. It is also seen that the influence of thermo-optic coefficient is dominant throughout the whole temperature range which may be due to some environmental effects in TiO2 ALD deposited coatings.

Fabrication of the resonance waveguide filters involves the control of aspect ratio of the structure in polymers is more challenging than inorganic materials. As the first demonstration the subwavelength replicated test structures in PC after
ALD deposition is shown in Fig 5. The vertical pillars seen in scanning electron microscope picture were due to bending effect generated in polycarbonate after cutting sample.

Fig. 3. (a) TM mode reflectance spectra of RWF at peak wavelength 633 nm with FWHM 3 nm, (b) Shows a shift of 0.2 nm/5°C towards longer wavelength due to contribution of TEC only, (c) Shows a shift of 0.4 nm/5°C towards shorter wavelength due to contribution of TOCs of TiO2 and PC only, (d) The wavelength shift is partially stabilized by combining (b) and (c) effects.

4. Conclusion

Resonance waveguide grating structures are designed for slightly above room temperature at a peak wavelength of 633 nm with a full width half maximum FWHM of 3 nm using transverse magnetic TM mode. A shift in peak wavelength towards longer wavelength was observed when only TEC is taken into account. The shift in wavelength was calculated at various temperature changes up to 100 °C and plotted to give almost linear approximation with a slope of 0.0422. In addition, another shift in wavelength was observed in the shorter wavelength region due to dominant influence of the TOCs of TiO2 and PC materials, showing a characteristic slope of 0.0673. Thus, partial athermalized devices can be
realized as a spectral combination of TEC and TOC effects with slope 0.02352 which is less than either TEC or TOC effects.

Fig. 4. (a) Effect of temperature on wavelength shift due to TEC only, (b) Effect of temperature on wavelength shift due to TOC only, (c) A comparison of TEC and TOC effects, (d) Combined TEC and TOC effects showing partial athermalization.
Fig. 5. A cut profile of polycarbonate grating test structure as partially athermalized RWF after ALD deposited TiO2 layer on PC.

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References