Micromechanical and microfluidic devices incorporating resonant metallic gratings fabricated using nanoimprint lithography

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Abstract. Optical filters based on resonant gratings have spectral characteristics that are lithographically defined. Nanoimprint lithography is a relatively new method for producing large area gratings with sub-micron features. Computational modeling using rigorous coupled-wave analysis allows gratings to be designed to yield sharp reflectance maxima and minima. Combining these gratings with microfluidic channels and micromechanical actuators produced using micro electromechanical systems (MEMS) technology forms the basis for producing tunable filters and other wavelength selective elements. These devices achieve tunable optical characteristics by varying the index of refraction on the surface of the grating. Coating the grating surface with water creates a 33% change in the resonant wavelength whereas bringing a grating into contact with a quartz surface shifts the resonant wavelength from 558 nm to 879 nm, a fractional change of 58%. The reflectivity at a single wavelength can be varied by approximately a factor of three. Future applications of these devices may include tunable filters or optical modulators.

Keywords: Nanoimprint lithography, surface plasmons, grating, optical filter, MEMS, electrostatic actuators, microfluidics.

1 INTRODUCTION

Wavelength selective filters are commonly employed in various devices for wavelength division multiplexing (WDM) such as optical add-drop multiplexers (OADM) and channel-select filters. Relative to multilayer dielectric optical filters, grating-based filters have the advantages that they require fewer thin-film layers. More importantly, since the grating characteristics are defined lithographically, filters with different optical characteristics (such as center wavelength) can be fabricated on the same substrate. Classical diffraction gratings, in which the incident light is angularly dispersed by wavelength, are widely employed in WDM systems. An alternative approach is to utilize resonant gratings in which the incident light is coupled into in-plane grating resonances. Depending on the characteristics of the grating structure, the resonance may result in either a reflectance maximum or minimum, allowing various types of add-drop and channel-select filters to be fabricated. The lack of simple electromagnetic models for the optical behavior of these resonant gratings and the difficulty of fabricating sub-micron grating features has limited the use of these structures to date. However, recent improvements in nanolithography and in the computational models for light propagation in periodic media [1] promise to reduce or eliminate many of the challenges in designing and fabricating resonant grating structures.

electromagnetic waves on the grating surface. A key feature of these resonances is that they occur when the angle of incidence and the grating period are chosen such that a propagating mode becomes evanescent. As a result, resonances are particularly apparent in gratings whose period is close to (or smaller than) the operating wavelength as such a grating may not support any propagating diffraction orders. Instead, the incident light is coupled into in-plane guided resonances. A variety of different structures based on dielectric films with periodically modulated refractive index have been demonstrated that exploit this effect, including 1-D subwavelength gratings [5] and 2-D photonic crystal slabs [6], as well as guided-mode resonant gratings (GMRG) [7, 8].

Wide interest in resonance phenomena in metallic gratings with subwavelength features was sparked in 1998 when Ebbesen et al. [9] reported extraordinary transmission of light through a metal film perforated with a periodic array of subwavelength holes. In this work, the zero-order transmission spectrum was found to contain several resonant peaks where the transmission magnitude is greater than the ratio of the hole area to the total surface area and several orders of magnitude larger than predicted by classical aperture theory. The source of this enhanced transmission is now understood to be the coupling of light into surface plasmons (SPs) by means of grating resonances. Similar resonance effects can be excited by inducing periodic variations in the refractive index on the surface of a metal film either by creating surface topography or by depositing a periodically patterned dielectric layer on top of the metal [10]. Maximum transmission efficiency occurs when the refractive indices of the superstrate and substrate are matched, as this condition results in identical resonant wavelengths on the top and bottom interfaces of the metal grating [10]. Even under this matched condition, absorption losses limit the transmission efficiency of a metallic grating. For this reason, we have investigated reflective metal gratings whose properties are dominated by resonances created on the upper surface of the metal.

Since lithography can be a costly process, gratings have long been fabricated by replication methods where a precision master grating is impressed into a polymer-coated plate. Replication techniques are likely to prove extremely important for the mass commercialization of nanostructured gratings. Serial techniques, such as electron-beam or focused-ion beam (FIB) lithography, are simply too slow and expensive for cost-effective production of large optical surfaces. In contrast, nanoimprint lithography (NIL) is fast, low cost, and has proven to be a viable lithography method to produce nanometer scale features [11, 12]. Since NIL requires contact between a master template and the substrate to be imprinted, it is more prone to defects than e-beam or optical projection lithography, but gratings are considerably more defect-tolerant than integrated circuit (IC) devices.

This paper concerns the combination of nanoimprinted resonant grating structures with micro-electromechanical systems (MEMS) technology. The relatively simple structure of resonant gratings makes them suitable for integration with a variety of MEMS devices including microfluidic flow channels and micromechanical MEMS actuators, as shown schematically in Fig. 1, thus allowing wavelength-tunable filters, optical modulators, and reconfigurable OADMs to be realized. Wavelength tuning can be accomplished by varying the grating period [13], the angle of incidence [14], or the index of refraction of the grating [15] or an adjacent layer [16]. We have chosen to investigate the latter approach, in which the resonance wavelength is controlled by varying the refractive index of the superstrate medium ($n_1$). Two approaches to induce refractive index changes are illustrated in Fig. 1. In the first approach, shown in Fig. 1(a), the grating forms the bottom surface of a fluid-filled channel. The fluid channel may be filled with liquid crystal (LC), allowing $n_1$ to be controlled with electric field. LC modulators [16] and tunable filters [17] that employ this technique have recently been demonstrated for the 1550 nm band. Larger changes in $n_1$ (and therefore larger wavelength tuning ranges) can be achieved by locally displacing the fluid in the channel with an air bubble manipulated by thermocapillary force [18]. In the second approach, shown in Fig. 1(b), the grating forms the surface of a MEMS actuator and $n_1$ is varied by mechanically
translating the grating in and out of contact with a dielectric substrate, allowing an optical modulator to be realized [19]. In comparison with the microfluidic and LC approaches, the micromechanical approach allows larger variations in refractive index to be achieved with fast (sub-millisecond) switching speeds. A relatively simple fabrication process can be used to fabricate an array of independently-addressed micromechanical pixels on the same substrate. Alternatively, sensitive measurements of grating displacement can be realized by monitoring the zero-order reflectance intensity [20] or by detecting changes in the resonance wavelength due to near-field coupling between two adjacent movable resonant gratings [21, 22].

Fig. 1. Cross-section views of grating-based devices. (a) Microfluidic device with a flow cell disposed over the grating surface. (b) Micromechanical device with grating fabricated on the surface of a MEMS actuator. The inset at the right shows a top view of an individual grating pixel suspended with micromechanical flexures.

2 PRINCIPLE OF OPERATION

Fig. 2(a) shows an illustration of a grating consisting of a metallic film perforated with an array of subwavelength holes. The grating structure consists of three layers, layer 1 (z > t) represents the dielectric superstrate above the grating, layer 2 (0 < z < t) represents the grating layer whose refractive index is periodically modulated along both the x and y axes, and layer 3 (z < 0) represents the dielectric substrate beneath the grating. The grating is illuminated with a plane wave from layer 1 which is diffracted by layer 2 into forward and backward propagating waves, representing the light transmitted and reflected by the grating, respectively.

By analogy to resonant circuits, a grating consisting of a metal film perforated with a periodic array of holes has been termed an inductive grating, whereas a grating consisting of periodically repeating metallic dots on a dielectric substrate is described as a capacitive grating [23]. Inductive gratings, like the ones described in this paper, are highly reflective at long wavelengths and display a reflectivity minimum (transmission maximum) at the resonance wavelength, whereas capacitive gratings have complementary characteristics and display a reflectivity maximum (transmission minimum) at resonance [24]. It is difficult to accurately calculate the resonant wavelengths with a simple analytical formula. Nevertheless, some intuition about the optical behavior of the grating can be developed from a simple kinematic model for the coupling of diffracted light into surface plasmon (SP) polaritons propagating on the metal surface [25]. This model assumes that resonance occurs at wavelengths where the SP wavenumber (k\text{sp}) matches the allowable grating wavenumbers,
where $k_x$ represents the in-plane wavenumber of the incident light, $\Lambda$ is the grating period, and $i$ and $j$ are integer indices. Neglecting the modulation of the metal surface, $k_{sp}$ for a smooth metallic surface is given by

$$k_{sp} = k_x \pm i(2\pi/\Lambda) \pm j(2\pi/\Lambda) ,$$  

(1)

where $\lambda$ is the free-space wavelength, $\epsilon_m$ is the complex permittivity of the metal, and $\epsilon_d$ is the complex permittivity of the dielectric. For insulators the imaginary component of $\epsilon_d$ is negligible [26]. Equations 1 and 2 can be combined to yield an estimate of the resonance wavelengths ($\lambda_{ij}$). Under normal incidence ($k_x = 0$),

$$\frac{\lambda_{ij}}{\Lambda} = \frac{1}{\sqrt{i^2 + j^2}} \sqrt{\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d}} .$$  

(3)

This calculation tends to underestimate the actual resonance wavelength since it was derived assuming a surface plasmon propagating on a smooth, unmodulated surface. Wood’s anomalies also produce sharp optical resonances that are located close to the SP resonances. The wavelengths of the Wood’s anomalies can be estimated from:

$$\frac{\lambda_{ij}}{\Lambda} = \frac{1}{\sqrt{i^2 + j^2}} \sqrt{\epsilon_d} .$$  

(4)

The SP resonances predicted by Equation 3 differ from the Wood’s anomalies predicted by Equation 4 by a factor of $\sqrt{\epsilon_m / \epsilon_m + \epsilon_d}$. For a highly conductive metal, this term is slightly greater than unity and the SP resonances are red-shifted with respect to the Wood’s anomalies. As an example, a silver grating in air ($\epsilon_d = 1.0$ and $\epsilon_m = -13.98 + 0.625i$, respectively) with a periodicity $\Lambda = 500$ nm has a Wood’s anomaly at $\lambda_{01} = 500$ nm and an SP resonance at $\lambda_{01} = 520$ nm.

More accurate estimates of the optical characteristics of these gratings can be made using computational models such as rigorous coupled-wave (RCW) and finite difference time domain (FDTD) analysis. We utilized a commercial software package (GD-Calc, KJ Innovation Software) which implements a version of RCW analysis known as the Fourier Modal Method (FMM). Models were produced for a silver grating with $\Lambda = 500$ nm, $a = 155$ nm, and $t = 100$ nm, as illustrated in Fig. 2(b). Due to limitations on CPU speed and memory, it is necessary to minimize the number of Fourier coefficients used in the analysis. As a convergence test, we computed the zero-order diffraction efficiency at a single wavelength ($\lambda = 542$ nm) versus number of Fourier coefficients. The calculated efficiency, shown in Fig. 3(a), increases in accuracy in an oscillatory fashion as the number of coefficients used in the calculation is increased. We found that complete convergence requires more than ten coefficients but five coefficients are sufficient to achieve convergence within $\sim$20% of the final value. This error is relatively small in comparison to the errors produced by variations between the model and the experimental gratings. The zero-order (specular) reflectivity was then calculated as a function of wavelength using five Fourier coefficients, as shown in Fig. 3(b). The resulting spectrum shows a sharp reflectivity minimum at $\lambda = 550$ nm, slightly red-shifted in comparison to the value predicted using Equation 3.
3 FABRICATION

The processes used to fabricate microfluidic and micromechanical devices are illustrated in Fig. 4. Each process begins with a nanoimprinting step in which the starting substrate is spin-coated with a 350 nm thick layer of polymethyl methacrylate (PMMA) (Fig. 4a). For microfluidic devices, we use standard 100 mm silicon wafers, while micromechanical devices were fabricated on 100 mm silicon-on-insulator (SOI) wafers in order to allow the selective release of micromachined pixels. The grating pattern is produced by thermal imprinting with a silicon template using a Nanonex NX-2000 nanoimprinter (Fig. 4b,c). The original template was fabricated using laser interference lithography [27] and consisted of a silicon wafer patterned with a one inch square array of 200 nm diameter, 300 nm tall SiO₂ posts, with a pitch of 500 nm. After imprinting, microfluidic devices are fabricated by directly metallizing the PMMA surface (Fig. 4d) and assembling a second chip with etched microfluidic channels on top of the grating chip (Fig. 4e). Low-cost microfluidic devices can also be fabricated by direct thermal imprinting into solid polymer slabs [28] rather than silicon wafers.

Micromechanical devices are fabricated by transferring the imprint pattern from the PMMA into the silicon device layer of the SOI wafer by plasma etching (Fig. 4f). Individual flexure-suspended silicon pixels are then patterned via optical lithography and deep reactive ion etching (DRIE), after which the pixels are released by using DRIE to remove the silicon handle wafer beneath each pixel (Fig. 4g). The surface of the silicon grating is then metallized by shadow evaporation at an angle of 45 degrees with respect to the wafer surface (Fig. 4h). During the evaporation process, the wafer is continuously rotated at 20 RPM, ensuring that the metal is deposited on the surface of the silicon and the periphery of the holes but not in the bottom of the holes. Finally, a fused silica wafer containing transparent indium tin oxide (ITO) control electrodes and a layer of insulating SiO₂ is assembled on top of the MEMS wafer (Fig. 4i). SEM micrographs of an etched silicon grating and a metallized PMMA grating are shown in Figs. 5(a) and 5(b), respectively. The resulting hole periodicity and diameter are 500 nm and 110 nm, respectively. Circular holes eliminate polarization dependent reflection and transmission characteristics reported for noncircular holes [29].

4 EXPERIMENTAL RESULTS

Completed gratings metallized with both aluminum and silver were tested with the use of an optical spectrometer (Ocean Optics USB2000) coupled to a microscope. Broadband light from a tungsten filament lamp was directed through the microscope onto the metal grating. Zero order reflected light was collected by the microscope objective and measured with the spectrometer. Fig. 6 shows measured reflectance spectra with the grating surface exposed to
dry air and coated with water along with reflectance spectra computed using RCW analysis. The analytical SP wavelengths calculated using Equation 3 with \((i,j) = (1,0)\) are marked with solid vertical lines. SP theory closely predicts the location of reflectivity maxima preceding reflectivity minima, which is in agreement with other reported results involving the interference of the reflected incident wave and surface waves [30]. Moreover, the resonant wavelength, modulation depth, and linewidth of the experimental spectra closely correspond to the spectra predicted by RCW analysis.

Fig. 4. Fabrication process: spin-coat PMMA (a), imprint (b), cool and separate template (c). For microfluidic devices, the grating is metallized (d) and a microfluidic channel is assembled on top of the grating (e). For micromechanical devices, plasma etching is used to transfer the imprint pattern into the silicon device layer (f), pixels are patterned and released (g), the grating is metallized (h), and a quartz wafer with ITO and SiO\textsubscript{2} is assembled onto the MEMS wafer.

Fig. 5. Scanning electron micrographs of completed gratings with \(\Lambda = 500\) nm and \(a = 150\) nm. (a) Grating pattern etched into a silicon substrate by RIE. (b) PMMA grating metallized with a 60 nm thick silver layer.
To ensure accuracy, both the analytical and RCW calculations were performed using measured values of the complex index of refraction for the metal (Ag and Al) films. Measurements were performed on unpatterned regions of the metal film with a spectroscopic ellipsometer (J. A. Woollam M-44). By measuring the refractive index, we account for any surface oxidation of the metal film. Note that the silver metallized grating displays a deeper reflectivity minimum than the aluminum grating. The average quality factor of the reflectance minimum was calculated by dividing the center wavelength by the full-width at half-maximum (FWHM) and was found to be 35.6 and 13.0 for the Ag and Al gratings, respectively. Several factors contribute to the difference in quality factors. First, Ag has a higher conductivity (and thus lower propagation loss) than Al. If the difference in quality factor were entirely due to metal conductivity, we would expect that the Ag grating would have a quality factor that is 4.7 times that of Al (equal to the ratio of the conductivities). Since the actual ratio of the quality factors is only 2.7:1, we believe that other device parameters play an important role in determining the quality factor. Among these parameters are the hole diameter, the metal film thickness, and scattering losses produced by surface roughness and aperture irregularities. The observation that the Ag film shown in Fig. 5(b) has large grains comparable in size to the subwavelength holes suggests that the scattering losses are significant in our current devices. We believe that we can improve the quality factor by reducing the surface roughness and by optimizing the device geometry using RCW analysis. Although we do not presently know the limit of achievable quality factor, using the ratio of metal conductivities as a guide we estimate that the quality factor of the Ag grating can be improved by more than a factor of two using this approach.

Fig. 6. Specular reflectance for (left) Ag grating and (right) Al grating with and without a fluid superstrate layer. Experimentally measured spectra are indicated with solid and dashed lines while spectra computed via RCW analysis are indicated with dash-dot lines. The resonance wavelengths predicted using surface plasmon (SP) theory are indicated by vertical lines. Average quality factors for the Ag grating and Al grating are 35.6 and 13.0, respectively. The resonant wavelength increases in proportion to the refractive index of the superstrate.

To demonstrate mechanical modulation of the grating reflectance, a high resolution spectrometer (Ocean Optics HR4000) was used to measure reflectance spectra of a silver metallized grating mounted beneath a quartz wafer. The spectra, shown in Fig. 7, were measured with the grating in contact with the quartz wafer and separated by a small air gap. When the grating and the quartz wafer are separated by an air gap greater than 500 nm, the spectrum displays a sharp reflectance minimum at \( \lambda = 558 \) nm. When the grating is in contact with the quartz superstrate, the resonance is red-shifted to \( \lambda = 879 \) nm, and the reflectance at \( \lambda = 558 \) nm is similar to that of an unpatterned metal mirror. The modulation depth at \( \lambda = 558 \)
nm is 60.7%. As with the fluid measurements presented in Fig. 6, the measured fractional wavelength shift ($879/558 = 1.58$) is nearly equal to the refractive index of quartz ($n = 1.54 @ \lambda = 879$ nm). At present, we do not understand why the modulation is relatively weak at $\lambda = 879$ nm. We note that the tungsten light source used in these measurements has relatively little output intensity for $\lambda > 900$ nm and we believe that this may reduce the accuracy of our long-wavelength measurements.

Fig. 7. Experimental measurements of specular reflection for a metallized grating in and out of contact with quartz superstrate. Out of contact is characterized as a separation greater than 500 nm between the quartz and the grating.

5 CONCLUSIONS

We have fabricated 2D metallic gratings using nanoimprint lithography. We showed that RCW analysis can accurately model the optical characteristics of the grating, facilitating the design of grating patterns to achieve a desired reflectance spectrum. Using standard MEMS fabrication techniques, these gratings are readily integrated with microfluidic and micromechanical structures. In turn, the MEMS structures allow the spectral characteristics of the grating to be controlled by modifying the refractive index of the superstrate. We have demonstrated two approaches to control the refractive index: by manipulating a liquid on the grating surface and by mechanically contacting the grating surface to a passive dielectric layer. Both techniques allow the resonance wavelength to be varied over a broad wavelength range. In microfluidic devices, we have measured a shift in the resonance wavelength from 550 nm to 725 nm ($\Delta \lambda / \lambda = 31\%$). In micromechanical devices, the reflectance at the resonant wavelength can be rapidly modulated, and we have measured a 60.7% change in the reflectance. Further process integration to produce controllable MEMS pixel elements will result in optical modulators and tunable filters for various communication and display applications. The ultimate wavelength tuning range that can be achieved using our approach is imposed by the refractive index of the superstrate materials employed. Liquids with refractive index approaching $n = 2$ are commercially available, but liquids with $n > 1.6$ are not colorless. For micromechanical devices operating at near-infrared wavelengths, a silicon ($n = 3.52 @ \lambda = 1550$ nm) superstrate would allow the resonance wavelength to be shifted by more than 300%. However, when a high-index material such as silicon is employed, reflections from the silicon-air interfaces are non-negligible and are likely to pose additional complications in device design (requiring the use of anti-reflective coatings, for example).
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