Bilayer Al wire-grids as broadband and high-performance polarizers

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Abstract: We have fabricated, characterized and theoretically analyzed the performance of bilayer (or stacked) metallic wire-grids. The samples with 100 nm period were fabricated with extreme-ultraviolet interference lithography. Transmission efficiency over 50% and extinction ratios higher than 40 dB were measured in the visible range with these devices. Simulations using a finite-difference time-domain algorithm are in agreement with the experimental results and show that the transmission spectra are governed by Fabry-Perot interference and near-field coupling between the two layers of the structure. The simple fabrication method involves only a single lithographic step without any etching and guarantees precise alignment and separation of the two wire-grids with respect to each other.

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1. Introduction

A perfect-conductor wire-grid transmits TM-polarized light (transverse magnetic; electric field perpendicular to the wires) and reflects TE polarization (transverse electric; electric field parallel to the wires) efficiently, provided that the wavelength of the incident light is much larger than the period of the grid. Subwavelength metal wire-grids are widely used in radio, microwave and IR region of the spectra [1]. With the development of nanolithographic methods, they are becoming available for the NIR, visible and UV regions and attracting increasing attention with increasing manufacturability [2-8]. They are an attractive alternative to conventional polarizers, since they are compact and planar and they have high performance providing high extinction ratios and transmittance and reflectance over a wide incident angle and wavelength range. Moreover, metal wire gratings are compatible with integrated circuit fabrication which facilitates the use of optical components such as polarizers, beam splitters, isolators, and wave plates in nanophotonic, fiber optic, display and detector devices [9-13].

Fabrication of metal wire-grids, where a single layer grating consisting of metal wires on an optically transparent substrate is aimed, mostly involves lift-off or reactive ion etching processes. In order to achieve high performance polarizers for the visible and UV ranges, high-aspect ratio metal grids are needed. Substantial progress has been made in recent years in developing metal gratings to operate down to UV/Visible range. For instance, an aluminum wire-grid polarizer with a period of 100 nm has been fabricated using nanoimprint lithography and reactive ion etching [3].

We have fabricated and characterized a new kind of wire-grid polarizer, namely bilayer metal wire-grids. The bilayer metal wire-grid can be considered, as shown in Fig. 1, as two metal gratings separated by a certain distance. We fabricated such structures by evaporating a metal film onto a photoresist grating. Since the fabrication process involves only photoresist patterning and metal evaporation, fabrication of bilayer metal gratings in this way is much simpler and less costlier than a single layer grating. As the final step is evaporation of the metal film, the fabrication process is self-masking, which means that defects on the nanostructured areas and unstructured areas that may exist on the substrate are automatically covered by an opaque metal film. Thus, the fabrication is robust against pinhole generation whereas in fabrication methods that incorporate metal etching or lift-off steps, defects can lead to pinholes. Such defects constitute one of the major limitations on the polarizing performance in particular when high extinction ratios are aimed.
In this paper we demonstrate through experimental results and theoretical analysis that metallic bilayer wire-grids can work as high-performance polarizers. Our findings show that the transmission of a bilayer wire-grid is strongly influenced by near-field coupling and Fabry-Perot type resonance between the layers. These effects lead to a polarizing performance that is better than a single layer wire-grid.

In related work, a bilayer metal-wire grid has been proposed as a reflective polarizer and a reflectance of about 50\% and an extinction ratio of about 200 have been realized for a narrow bandwidth, at a wavelength of about 650 nm [2]. Enhanced transmission through corrugated films has recently been demonstrated wherein the transmission is mediated by surface plasmon polariton (SPP) resonances [14]. In the present case, however, SPP resonances are not thought to be responsible for the high transmission, since the period of the wire-grid is considerably smaller than the wavelength [13].

The paper is organized as follows. In Section 2 the fabrication process of bilayer aluminum wire-grids is described in detail. Measurements of the transmission spectra are then presented in Section 3. The finite-difference time-domain (FDTD) simulation results are presented and compared with the experimental measurements in Section 4. The transmission mechanisms and the effects of near-field coupling and Fabry-Perot resonances on the transmission are also discussed in this section. The paper closes with a summary of major conclusions and outlook in Section 5.

2. Fabrication of Bilayer Wire-Grids

A series of different aluminum bilayer wire-grids with a period of 100 nm were fabricated on quartz substrates with different duty cycles, photoresist thickness and metal thickness. Polymethylmethacrylate (PMMA) films with thickness between 90-130 nm were spin-coated on quartz wafers. EUV interference lithography (EUV-IL) was used to create binary line/space type gratings in the photoresist. The EUV-IL facility at the Swiss Light Source (SLS) where the exposures were done, uses 13.4 nm EUV light generated by an undulator source. Two transmission diffraction gratings with equal periods were used to create and record a one-dimensional interference pattern on the substrate [15]. EUV-IL is a high-resolution, high-throughput method which enables fabrication of periodic nanostructures with periods well below 100 nm over large areas of several square millimeters with typical exposure times of only about 10 s.

Following the EUV exposure, the PMMA films were developed in an MIBK:IPA=1:3 solution for 45 s, to obtain the line/space patterns. Gratings with duty cycles changing between 0.3 and 0.5 were achieved by adjusting the exposure dose. Thermal evaporation of aluminum
was performed at normal incidence at a pressure better than $1 \times 10^{-6}$ mbar. The metal thickness ranged between 20 to 90 nm. The typical size of the gratings was $0.5 \times 6 \text{ mm}^2$.

A schematic cross section of a bilayer wire-grid is shown in Fig. 1. As mentioned above, thermal evaporation of aluminum onto the binary photoresist pattern results in two gratings which are separated from each other by a precise distance. The separation $d$ is determined by the photoresist thickness $h$ and the metal thickness $t$. The duty cycle of the two metal gratings, i.e. the ratio of the wire width to the period, is defined by the duty cycle of the underlying photoresist pattern, $f$. The upper grating has the same duty cycle as the photoresist whereas the lower one has a duty cycle of $1-f$. The diagram in Fig.1 depicts a rather idealized picture of the structures. In reality, as the film growth progresses the upper layer gets broader and the lower metal layer gets thinner, due to the shadowing effect. This is evident in the SEM cross-section shown in Fig. 2. The top-down image in the same figure mainly shows the Al lines of the upper layer.

![Cross-sectional and top-down images of a subwavelength aluminum bilayer wire-grid.](image)

**3. Polarization Measurements**

The transmission spectra were recorded using a Perkin-Elmer UV/Vis/NIR spectrometer in the 310-860 nm wavelength range with a spectral resolution of 2 nm at normal incidence. The measured spectra were smoothed over 10 nm by the Savitzky-Golay method. A depolarization unit before the sample chamber and a Glan-Thompson type polarizer after the sample chamber were installed in the spectrometer. Thanks to the large area of the samples no focusing optics was required. The spectra were measured with a fixed sample setup. First, the relative orientation of the tested wire-grid and the Glan-Thompson polarizer was determined by rotating the polarizer and minimizing the transmission. The spectral response of the sample was measured for the TE mode in this configuration in which the TE axis of the wire-grid is assumed to be parallel to the polarizer axis. Then the polarizer was rotated by 90° and transmission spectrum for the TM mode was measured.

The transmission spectra for the TM and TE modes and the extinction ratio of a typical sample are shown in Fig. 3. The TM transmission is at a constant level of about 45% at long wavelengths. The extinction ratio is over $10^4$ at 700 nm which is at the limit of our experimental precision. TE transmission tends to go up with decreasing wavelength. This is consistent with the optical properties of aluminum, since with decreasing wavelength its...
complex refractive index – both the real and imaginary parts decrease and thereby the metal moves farther away from being similar to a perfect conductor. The slight increase of the TE transmission above 800 nm is attributed to the interband transitions of aluminum which locally reverse the general trend of the refractive index as a function of the wavelength [16].

Fig. 3. Measured transmission spectra and extinction ratio of an Al bilayer wire-grid with \( p=100 \text{ nm}, \ h=94 \text{ nm}, \ t=60 \text{ nm}, \) and \( f=0.36. \)

4. Theory and Discussion

We used finite-difference time-domain (FDTD) calculations [17] to simulate the optical response of the bilayer grids. The geometry of the simulation cell is shown in the right-most column in Fig. 4. The wires lie parallel to the y axis and the simulation domain is in the xz plane. Periodic boundary conditions for the x and y axes are employed. A monochromatic plane-wave is sent onto the bilayer grating from the top in the +z direction. The transmitted wave propagates further along the z axis into the quartz substrate. The simulation was run until the steady state was reached in the transmitted field amplitudes. Note that in this method separate simulations were run for each wavelength, where we used the corresponding optical constants of the materials. Absorbing boundary conditions at both ends of the cell along the z axis are realized by the use of perfectly matched layers (PML) [18] which guarantee negligible reflection at these boundaries. The geometrical parameters are set to the same values as the sample in Fig. 3. For the optical constants of aluminum, the values based on reflectance data on clean and unoxidized films prepared and measured in UHV are used [16]. For simplicity, the natural oxide layer on the aluminum surfaces is not taken into account.

In Fig. 4, the amplitudes of various field components calculated for a 300 nm-wavelength incident beam are shown. Due to the invariance of the structure along the y axis, the TM mode, consisting of the field components \( E_x, H_y \) and \( E_z \), and the TE mode, consisting of \( E_y, H_x \) and \( H_z \), are completely decoupled. The E-field of the incident wave was set to have equal amplitudes in the x and y directions. As seen in the figure, while a significant amount of \( E_x \) is transmitted through the bilayer grating, \( E_y \) is mainly reflected and decays rapidly between the metal wires of first layer because the spacing between the wires, that is smaller than \( \lambda/2 \) does not allow the propagation of TE modes [19]. The small amount of transmitted \( E_y \) through the upper grating is damped further by the lower grating.
Fig. 4. The profiles of the electromagnetic field amplitudes ($|E|$ and $|H|$) at $\lambda=300$ nm passing through an Al bilayer wire-grid with $p=100$ nm, $h=94$ nm, $t=60$ nm, $f=0.36$. The geometry of the simulation cell is shown in the right-most column. The refractive indices of aluminum, quartz, and PMMA are taken as $n=0.276+3.61i$, $n=1.46$ and $n=1.48$, respectively. The amplitudes are plotted with linear scale where the minima are set to zero and the maxima are set to maximum amplitudes of the individual field components.

The transmittance of the grating for both TM and TE modes can be defined as

$$T = \frac{|E_t|^2}{|E_i|^2} \cdot n_q,$$

where $E_i$ and $E_t$ are the amplitudes of the electric fields of the incident and transmitted waves and $n_q$ is the refractive index of the quartz substrate. $E_i$ is the predefined amplitude of the excitation signal. $E_t$ is found by determining the electric field ($E_x$ or $E_y$) well below the grating where near-fields are negligible and $E_x$ and $E_y$ are constant along the x and z axes. At a distance of 150 nm below the grating the field amplitudes are constant within an error of less than 1%.

In Fig. 5, the calculated transmittance of both TM and TE modes and the extinction ratio are plotted as a function of the wavelength. Since our exploratory simulations revealed that the transmission is rather sensitive to the cross-section of the bilayer grating and the actual cross-section of the structures are complicated (see Fig. 2), for comparison we used two different approximations to model the cross-section. Fig. 5a shows schematic diagrams of a simplistic (model-A) and a more realistic (model-B) cross-section. Fig. 5b compares the calculated transmission in the TM mode with the measured values. The TM transmission for model-A agrees rather well with the experiment at wavelengths above 600 nm. However below 600 nm...
it diverges significantly from the experimental curve. The TM transmission for model-B seems to follow the general trend of the experimentally measured spectrum except for a 10-15% offset over the whole spectral range. Both curves show a relatively flat region above 600 nm and a gradual decrease below this wavelength with similar slope. The calculated TE transmission values plotted in Fig. 5c show trends similar to the experimentally measured one. However, the calculated values are lower than the experimental ones by a factor of about 5 for model-A and by a factor of about 3 for model-B. Fig. 5d compares the extinction ratios where the main trends of the curves as well as the differences between them are mainly determined by the TE transmission.

The differences between the experiment and the theory (in both TM and TE modes) can be attributed to the simplifications of the model regarding the cross-sectional profile of the grating and the natural oxide layer of aluminum. In particular, the dependence of the spectral behavior on the grating profile is clearly seen in the two model systems that we simulated as explained in the preceding paragraph. In addition, there are some other factors which should contribute to the large difference between the calculation and experimental results for the TE mode. Although the fabrication process is robust against pinhole generation and inspection under the optical transmission microscope revealed no detectable pinholes, this cannot be completely ruled out. The background signal of the detector and leakage of the TM intensity due to the adjustment error of the azimuthal angle can also contribute to the measured TE transmission particularly for very low transmission rates. Moreover, the roughness of the

Fig. 5. Calculated transmission spectra and extinction ratio of an Al bilayer grating with \(p=100 \text{ nm}, h=94 \text{ nm}, t=60 \text{ nm}, f=0.36, \) (a)The schematic diagrams of the cross-section models used in the calculations. The comparison of the TM transmission (b), TE transmission (c), and extinction ratio (d) for the two cross-section models and experiment.

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aluminum lines and other defects which act as point scatterers can increase the TE transmission.

In order to gain deeper insight into the transmission of light through bilayer gratings we carried out further simulations where we changed the geometrical parameters of the bilayer grating. The investigation of the influence of these parameters should help in further improvement of the performance of the bilayer gratings. The effect of the separation between the two layers on the transmission efficiency is shown in Fig. 6 for the wavelengths of 700 nm and 300 nm. In these and the following calculations the rectangular cross-section model (model-A, Fig. 5a) is used. The duty cycle is set to \( f = 0.5 \), which generally leads to the most efficient transmission of TM mode. The metal thickness is set to \( t = 90 \) nm, which according to our simulations, provides extinction ratios comparable to the best available polarizers such as Glan-Thompson and Wollaston type crystal polarizers. The photoresist and the substrate are omitted in these calculations as they have small effects on the transmission properties but can complicate the analysis of the effects of other structural parameters.

The results of the FDTD simulation of the bilayer grating are shown with symbols in Fig. 6. The solid lines in this plot, however, were calculated with a different approach which we shall discuss below. As seen in the figure both the TM and TE transmissions are dominated by strong oscillations that are reminiscent of a typical Fabry-Perot (FP) interferometer. This can be explained by considering that the light transmitted through the first grating is partially reflected by the second grating and it travels back and forth between the two gratings leading to constructive or destructive interference at certain separations. Such resonances were reported for periodic slit arrays in thick metal films wherein the reflection occurs at the slit openings [20, 21]. The resonance behavior that appears in Fig. 6 in our analysis is due to the FP cavity formed by the two gratings. It is likely that there are interference effects within the layers in our gratings but these are not apparent in Fig.6 as the grating thickness is not varied in these calculations.

To confirm the FP resonance we modeled the bilayer grating by two interfaces. The transmission of a FP interferometer formed by two identical interfaces is given by [1]

\[
T = \frac{T_0^2}{1 + R_0^2 - 2R_0 \cos[\delta]}, \tag{2}
\]

where \( T_0 \) and \( R_0 \) are the transmittance and reflectance of the interface and

\[
\delta = m \frac{4\pi d}{\lambda} + 2\phi. \tag{3}
\]

Here, \( d \) is the distance between the interfaces, \( \phi \) is the phase change of the incident wave upon reflection and \( m \) is an integer. We carried out FDTD simulations of a single layer grating and determined the values of \( T_0, R_0 \) and \( \phi \) for both TM and TE modes. The obtained parameters are listed in Table 1 for \( \lambda = 300 \) nm and 700 nm. The transmission efficiency based on Eq. (2) and the parameters in Table 1 are plotted as solid lines in Fig. 6. As seen in the plot, the FP model is, in general, in excellent agreement with the “full FDTD simulation” of the bilayer grating. However full FDTD results (symbols), tend to deviate from the FP model (solid lines) at separation distances below 20 nm and 70 nm for the wavelengths of 700 nm and 300 nm, respectively. We attribute this deviation to the near-field coupling between the two layers as we show below in simulations designed to accentuate the near-field effects.
Fig. 6. Calculated transmission spectra and extinction ratio of an Al bilayer grating as a function of separation between the layers at the incident wavelengths of (a) $\lambda=700$ nm and (b) $\lambda=300$ nm. $d=h-t$, $p=100$ nm, $r=90$ nm, $f=0.5$. In this calculation the photoresist and the quartz substrate are omitted. The scattered data points are the results of the simulations of a bilayer wire-grid whereas solid lines are calculated by using Eq. (2) and the values listed in Table 1. In the insets TE transmission spectra are plotted with higher magnification.

Table 1. The calculated transmittance ($T_0$), reflectance ($R_0$) and phase change upon reflectance ($\varphi$) of a single layer Al wire-grid at wavelengths of 700 and 300 nm for TM and TE polarization. $p=100$ nm, $r=90$ nm, $f=0.5$.

| $\lambda$ [nm] | Polarization | $T_0$   | $R_0$   | $\varphi$ [rad] |
|----------------|--------------|---------|---------|-----------------|
| 700            | TM           | 0.76    | 0.19    | -3.55           |
| 700            | TE           | 2.6x10^-4 | 0.87    | -2.75           |
| 300            | TM           | 0.85    | 0.05    | -2.18           |
| 300            | TE           | 2.7x10^-3 | 0.89    | -2.20           |
One can imagine that if there is a near-field coupling between the two layers, this should have some dependence on the relative lateral positions of the wires in the two layers. In order to check the validity of this hypothesis we performed simulations where the two wire gratings are moved relative to each other laterally while the separation $d$ is kept constant, as schematically shown in the inset in Fig. 7. The transmission efficiency as a function of the lateral shift, $\Delta x/p$, for two different separations and for $\lambda=700$ and 300 nm is plotted in Fig. 7. In order to distinguish the effect of the near-field coupling from the FP resonance, we performed the simulations for a separation of 20 nm, where the near-fields are expected to be pronounced, and for a separation of $20 \text{ nm} + \lambda/2$, where the near-fields are negligible but the FP effect is the same. As expected, at large separation distances the lateral shift along the x axis has no effect on the transmission efficiency for both TM and TE modes at both wavelengths. This proves that at large enough separations there is no near-field coupling and the bilayer wire-grid works purely as a FP interferometer. In contrast, when the layers are separated by only 20 nm, the TE transmission depends strongly on the lateral shift. It decreases by about a factor of two for both incident wavelengths as the shift $\Delta x/p$ is changed from 0 to 0.5. In the latter extreme, the evanescent fields that go through between the wires of the first grating are blocked efficiently since the second grating is out-of-phase with respect to the first one. In terms of the performance of a polarizer this corresponds to a higher extinction ratio. At $\lambda=700$ nm the TM transmission decreases by only 2% when the gratings become out-of-phase. On the other hand, at $\lambda=300$ nm, TM transmission increases by 20% under the same conditions. These results show how the near-field coupling significantly alters the TM without necessarily enhancing it. Therefore, it is difficult to predict qualitatively the net effect of near-field coupling on transmission which depends on the detailed nature of the coupling controlled by the structural parameters and optical constants of the materials.

Having gained insight into how two gratings that are separated from each other by a precise distance work together, it is interesting to compare how such a system fares against two alternatives in terms of the relevant performance criteria. To this end, the polarizing performance of three different cases at $\lambda=300$ nm and 700 nm are compared in Table 2: A single layer wire-grid; a bilayer wire-grid; and two bi-layer wire-grids used in a tandem configuration where the spacing is much larger than the coherence length. The transmission efficiency of the tandem positioned grids is given as $T_T^2$, where $T_0$ is the transmission of a single layer wire-grid. Thus, two polarizers in tandem have a reduced transmission but higher extinction ratio. As seen in the table, the extinction ratio of the bilayer polarizer is better than the tandem configuration at both wavelengths. Furthermore, the transmission efficiency of the bilayer polarizer is higher than the tandem polarizers at both wavelengths and it is even higher than the single layer polarizer at 700 nm.

| $\lambda$ [nm] | Polarizer      | Transmission | Ext. ratio |
|----------------|----------------|--------------|------------|
| 700            | Single layer   | 0.76         | 2.9x10^4   |
|                | Bilayer        | 0.80         | 1.9x10^7   |
|                | In tandem      | 0.58         | 8.5x10^6   |
| 300            | Single layer   | 0.85         | 315        |
|                | Bilayer        | 0.74         | 5x10^7     |
|                | In tandem      | 0.72         | 9.9x10^4   |
Fig. 7. Calculated transmission spectra and extinction ratio of the Al bilayer grating as a function of the lateral shift between the layers at the incident wavelengths of (a) $\lambda = 700$ nm and (b) $\lambda = 300$ nm. The definition of lateral shift is visualized in the inset. Note that $\Delta x/p = 0.5$ corresponds to a bilayer grating as depicted in Fig. 1. $p = 100$ nm, $t = 90$ nm, $f = 0.5$.

Note that in the present study we did not carry out a systematic optimization of structural parameters for more efficient transmission. But still transmission efficiency above 80% was calculated for certain wavelengths and grating separations. The grating separation allows the tailoring of the FP resonance and near-field coupling. Further enhancement of the transmission should be possible by manipulating the FP resonance within the grating by changing the metal thickness [20, 21]. In general, we can expect to improve the extinction ratio by increasing the metal thickness. Moreover, antireflective coatings can be introduced in the polarizer design to improve the efficiency and to provide better handling and environmental durability [5]. If the range of interest is only visible or NIR, aluminum can be replaced by silver or gold for better performance. Reducing the period of the grating is expected to increase the polarizer performance for shorter wavelengths.
5. Conclusions

We have demonstrated that bilayer subwavelength metallic-wire grids work as high transmission and extinction ratio polarizers. The transmission mechanism is significantly affected by interference resonances and near-field effects between the two grating layers. A bilayer wire-grid polarizer is not only simple to fabricate, but also can be tuned to have better performance than a single layer wire-grid polarizer and two single layer wire-grid polarizers used in tandem.

Transmissions as high as 50% and extinction ratios above 40 dB were observed with fabricated bilayer Al wire-grids in the visible range in accordance with the theory. The presented simulations provide insight into the working principles which should help in the design of bilayer gratings. The simulation results show that transmissions over 80% and extinction ratios higher than 70 dB are achievable with plenty of room left for improvement through optimization of structural parameters and the use of additional films such as anti-reflection coatings. The deposition process should be tuned to obtain smooth films for best-possible performance. For better durability and higher aspect ratios the photoresist pattern can be transferred into the substrate with an etching process before metal deposition.

Although, we used EUV-IL lithography to pattern the photoresists in the present work, it can be replaced by low-cost and high-throughput methods such as laser interference lithography [22] or nanoimprint lithography [3]. The fabrication of the bilayer gratings involves only one lithographic step and it can be integrated into the currently used wafer-based semiconductor technology. The fabrication process is simple and applicable to large volume production. It guarantees precise alignment and separation of two wire-grids with respect to each other. Thus, bilayer gratings can find a wide area of applications with their high performance, low-cost manufacturability and IC technology-compatible fabrication.

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