RIGOROUS COMPUTATION AND FABRICATION OF 2D-SUBWAVELENGTH RESONANCE STRUCTURES FOR PHOTONIC APPLICATIONS

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Abstract

The use of metal 2D-SubWavelength Structures (SWS) is a promising solution for all those applications where a selective emission from a thermal source is desirable, e.g. photovoltaic and black-body emission. The investigation of the SWS' photonic bandgap properties is challenging, especially for the infrared and visible spectrum, where the fabrication difficulties have always represented an obstacle. In this paper, the anodization of aluminum films as a self-assembly method for the SWS fabrication is proposed. A rigorous calculation of 2D-SWS of gold having high-absorptivity in the visible and low-one in the NIR, their fabrication by DC-sputtering deposition through anodic porous alumina templates, and their optical and topographic characterization are presented.

Key words: SubWavelength Structure, Kirchhoff's law, absorption, Maxwell equations, rigorous coupled wave analysis, diffraction order, self-assembly structures, sputtering, porous alumina template.

Introduction

The Kirchhoff's law of radiation states that at the thermodynamic equilibrium and for a specific wavelength a physical body absorbs and emits the same electromagnetic energy. Considerations of this, awoke the interest in the metal Sub-Wavelength-Structures (SWS) in order to develop more efficient incandescence light sources, thermophotovoltaic elements [1,2], or selective Anti-Reflective (AR) surfaces to contribute to the energy saving. In other words, a SWS can selectively act on the emission spectrum of a thermal source to enhance the visible emission rate against the IR one. A result of this work is to prove the existence of a metal 2D-SWS which exhibits a resonance sharp absorption/emission change between the visible and the Near Infra-Red (NIR) parts of the EM spectrum. Two different gold SWS typologies have been theoretically analyzed, and their optical behavior presented by reporting calculated spectral reflectivity curves. A first type is here represented by a structure made of columns placed on a flat surface, and a second one is defined by holes; in both cases, columns and holes are arranged in a rhombic symmetry. Self-assembly techniques were analyzed and developed to fabricate column-type SWS; in particular, a 2D-SWS was made by DC magnetron sputtering deposition of gold into the nano-channels of Anodic Porous Alumina (APA), here used as a self-assembled template. Electron microscopy images and spectral reflectivity measurements of the fabricated 2D-Au-SWS are reported here. The spectral reflectivity curve exhibits a sharp fluctuation at the visible spectrum end.

Rigorous calculation of 2D-SWS

2D-SWS behave differently from the classical diffractive elements. In case of normal incidence, a SWS allows only the 0^{th}-diffraction order to be reflected, while all the others are evanescent; if the angle of incidence increases, few other orders can be reflected off the structure (Fig.1).

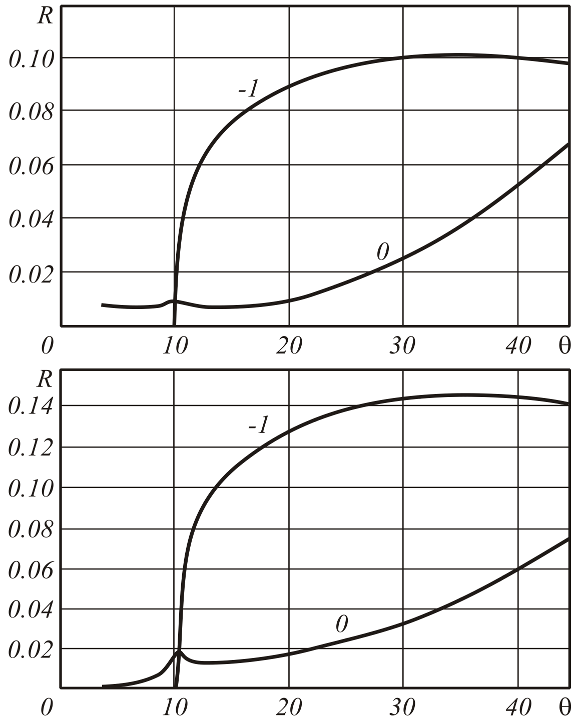

Figure 1. In this figure, reflectivity curves of single diffraction orders produced by a beam of wavelength 550nm are reported here for two particular square symmetry 2D-SWS of tungsten, and against the beam angle of incidence. Reflectivity is defined like the percentage of the incident beam energy reflected by the structure.
a) A SWS made up of 0.33λ deep square holes of side: 0.75d (where d is the structure period);
b) A SWS made up of 0.38λ deep circular holes of radius: 0.4d (where d is the structure period and λ is the wavelength).
In both cases, when the incidence angle is higher than 10 degrees, -1^{st} diffraction order is not evanescent anymore but it is reflected by the structure

This behavior makes SWS particularly suitable to confer antireflective properties to materials normally highly reflective in the visible-NIR range for thermal emission applications. The design of a SWS consists of searching for the parameters which define the structure profile, from the condition that the 0[th]-reflected order intensity is minimal. The 2D-SWS study, because of the features size involved (below the design wavelength), requires the rigorous calculation of the Maxwell equations [3-5], while neither the scalar approximation, valid for bigger periods, nor the effective medium theories are accurate.

The optimal parameters which define the structure profile can be calculated from the spectral optical behavior one wants the SWS to have, from the material physical properties, and in particular, the spectral dependency of its refractive index on wavelength at the working temperature. For these reasons, it is always preferable to deal with a material whose spectral reflectivity, $R(\lambda)$ is as close as possible to the desired one. To solve the electromagnetic problem in our case, the rigorous coupled analysis (RCWA) proposed by Moharam et al. was used [3]. Tne correct rules for the Fourier decomposition of the functions product were also realized [4,5].

The Kirchhoff's law states that the spectral emissivity of a surface, ε coincides with its spectral absorptivity, α; since $R=1-\alpha$, where spectral reflectivity is high, the correspondent emissivity is low and vice versa. The dependency of R, ε, and α on wavelength and temperature has to be kept into account as well. In this paper, spectral reflectivity curves are presented as a proof of the concept, either for the bulk material or for the nano-structured one; these curves were calculated considering the beam reflected by the SWS over the whole solid angle, the same curves which can be obtained by measuring reflectivity through an integrating sphere. A thorough analysis of the spectral reflectivity of different absorbing material brought attention to gold, silver and copper, which naturally exhibit a sharp reflectivity fall right in the middle of the visible spectrum. In figure 2, the calculated spectral reflectivity curves corresponding with two types of 400nm period 2D-Au-SWS are shown; a first type is made of 320nm diameter cylindrical pillars, 80nm spaced from each other (2D-Au-SWS-1), and a second one (2D-Au-SWS-2) is made of 320nm diameter cylindrical holes, 80nm spaced from each other of the same rhombic geometry. Each curve of figure 2 represents at a time both structures types when the 2D-Au-SWS-1 pillar height is equal to the 2D-Au-SWS-2 hole depth. In figure 2, spectral reflectivity curves calculated over the whole solid angle, for an angle of incidence equal to 8°, and for gratings made up of pillars/holes of height/depth ranging between 50 and 1000nm are reported. As one can see from figure 2, non-structured gold exhibits a reflectivity fall from 95 to 40% between 650 e 475nm respectively, and the bigger the pillar-height/hole-depth (up to 300nm) the more spectral reflectivity decays, sharper and sharper up to 10% is reached; furthermore, the bigger the SWS feature height/depth, the more said decay moves towards higher wavelengths; when pillar-heights/hole-depths are of the order of the visible wavelengths, from 500nm upwards, the migration of the reflectivity cut-off slows down until stopping at around 1 micron. The presented results show that the designed 2D-Au-SWS of pillar-heights/hole-depths ranging from 700 nm upwards, exhibit a quasi-total absorption over 800-650 nm, and above this spectral range, reflectivity decays from 80 to 9%.

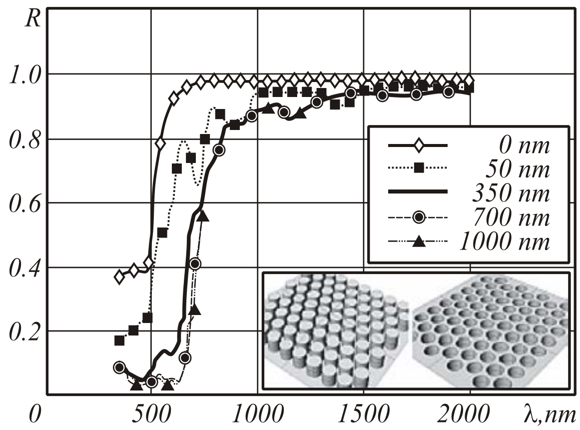

Figure 2. Calculated spectral reflectivity curves, $R(\lambda)$. Each pictured curve corresponds with a 2D-Au-SWS-1 and a 2D-Au-SWS-2, whereas the pillar height of the first type structure is equal to the hole depth of the second one. Each curve corresponds with a specific feature height/depth

In order to fabricate high efficiency incandescence light sources, gold can be used as well as tungsten. If gold is nano-structured according to the designed 2D-Au-SWS profiles a very high ratio between visible and infrared emission can be achieved; as a result, the element can be operated at a temperature lower than the gold melting point (1336ºK) with a consequent reduction of the convection and conduction losses; although new technological skills can be made up to avoid the profile deformations at working temperatures as high as 2800ºK, where the visible emission efficiency can be much higher than the conventional tungsten bulb one.

Fabrication of 2D-SWS of gold

In this work, an alternative way to fabricate 2D-SWS starting from self-assembled templates is presented, in particular APA is used as a mask. APA templates were prepared according to the standard technique of double anodization in 0.3M phosphoric acid, starting from one micron thick aluminum films [7]. The templates were fabricated to have 320nm diameter holes distributed in a rhombic symmetry and spaced 80nm from each other. The pore size and thus the grating duty cycle was changed by using pore widening techniques. Gold was infiltrated into APA nano-sized channels by DC-biased-magnetron sputtering in order to copy the APA template profile. Gold was infiltrated little by little in a number of identical sputtering steps, into the APA matrix channels placed 15 cm apart from the sputtering source on a 10 mm diameter circular glass substrate. Figure 3 shows SEM images of the fabricated 2D-Au-SWS. Sputtering deposition resulted in being a feasible way to infiltrate nano-porous templates alternative to the standard electrodeposition and CVD techniques [8].

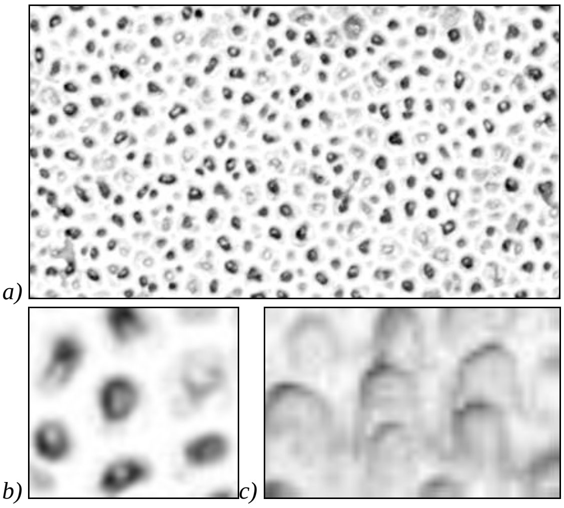

Figure 3. SEM images of the fabricated 2D-Au-SWS. The images show a rhombic symmetry 2D-Au-SWS made up of pillars 700nm high, spaced about 150nm from each other and of 250nm diameter circular base.
a) top view, wide area;
b) a detail - a top view and a 3D-image

Experimental measurements: spectral reflectivity

The experimental reflection spectra of the fabricated 2D-Au-SWS were measured through an integrating sphere by a visible-NIR spectrophotometer (the Cary 500 by Varian) over a spectrum ranging from 350 to 2000nm and with a lighting beam angle of incidence of 8°; the reported calculations were made according to the measurement set up. The integrating sphere aperture is about 75mm^2, therefore, only wide area samples could be hosted and measured, as a consequence, high uniformity samples had to be fabricated. Figure 4 shows the comparison between the calculated spectral reflectivity of a 2D-Au-SWS-1 made up of 700nm high pillars and the measured one, relative to the 2D-Au-SWS made of 700nm high, and 250nm diameter cylindrical pillars, spaced about 150nm from each other.

Looking at figure 4 it is apparent that the spectral position of the measured reflectivity fall coincides with the calculated one. Nevertheless, there are still important differences between the calculated and measured curves, which are probably due to the sample geometry being not exactly the same as the simulated one (pillars are rounded on top). As one can see in figure 3, the manufactured 2D-SWS geometry is not very uniform over a wide area, the grating filling factor does not correspond exactly to the desired one, but the period correspondence is good. The filling factor of the 2D-Au-SWS-1 is 62% average ($ff_{2D\text{-}Au\text{-}SWS}$ = pillar diameter/period) against the 80% average of the APA template (ff_{APA} = pore diameter/period).

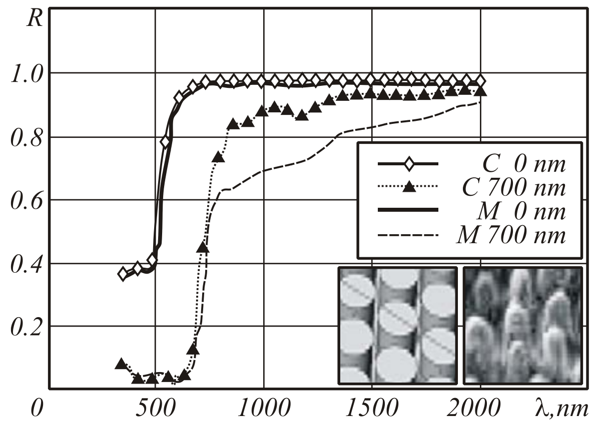

Figure 4. Spectral reflectivity curves. C-curves represent the reflectivity calculated by 7th order-RCWA, while M-ones are measurements. -The diamond marked curve is the calculated reflectivity of a gold flat surface, while the non-marked bold line is the relative measured curve. - Line marked with triangles shows the calculated reflectivity of a 2D-Au-SWS-1 made of 700nm high pillar. - The dashed line curve is the measured reflectivity of the 2D-Au-SWS prototyped

The most important significant deviation between theory and experiment is from 760nm upwards; in fact, in this spectral region, the measured reflectivity does not increase up to the predicted value; the experimental curve reaches only 60% and keeps increasing slowly and almost linearly. Aside from the mentioned geometrical mismatch, another possible deviation factor might be found in a possible disagreement between the gold optical constants used in the design and the real ones concerning the sputtered metal [9].

Conclusions

The use of a 2D-SWS represents a powerful method to change the spectral emission properties of an absorbing medium. Such structures allow the control of the spectral properties at the interfaces between different materials, and can be an important tool to improve the efficiency of incandescence light sources as well as solar and TPV cells [1,2,10]. In the present work, two different typologies of 400nm period 2D-SWS of gold were designed; a first type is made of pillars and a second one of holes placed on a flat surface. In both structures, pillars and holes have a 320nm diameter circular base arranged in rhombic symmetry; both structures exhibit a sharp reflectivity change between 625 and 800nm, where emissivity passes from 80 to 20%; it is besides sufficient to go up to 1100nm to observe emissivity equal to 90%, to get to 94% at 1400nm. An fundamental result of this work is the fabrication of 2D-SWS by infiltrating 320nm wide channels of APA by DC magnetron sputtering down to a depth of 700nm. Calculated and measured spectral reflectivity curves of a fabricated sample which show a satisfactory accordance between theory and experiment are reported here.

Acknowledgements

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<u>Key words:</u> SubWavelength Structure, Kirchhoff’s law, absorption, Maxwell’s equations, rigorous coupled wave analysis, diffraction order, self-assembly structures, sputtering, porous alumina template.

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