A FEASIBILITY STUDY TO DETERMINE AND VERIFY THE EFFECTIVE PERMITTIVITIES OF A SUBWAVELENGTH METALLIC PERIODIC STRUCTURE

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Effective medium theory (EMT) has been proposed to estimate the optical characteristics of periodically structured devices by analytically obtaining an approximate effective index of a periodic structure. According to the EMT, a periodic structure may be replaced with an artificial anisotropic homogeneous medium on condition that zeroth diffraction order propagates with evanescent higher diffraction orders and the structure is sufficiently thick such that the incident light does not propagate through. A simple second-order expression in a closed form provides an effective index of a periodic structure in the quasi-static limit, also known as long-wavelength limit, of $\Lambda << \lambda$, with Λ and λ being respectively grating period and free-space wavelength of incident light[1]. Namely,

$$\begin{aligned} \varepsilon_{eff,TE}^{(2)} &= \varepsilon_{0,TE} + \frac{\pi^2}{3} f^2(1-f)^2(\varepsilon_A - \varepsilon_B)^2 \left(\frac{\Lambda}{\lambda}\right)^2 \\ \varepsilon_{eff,TM}^{(2)} &= \varepsilon_{0,TM} + \frac{\pi^2}{3} f^2(1-f)^2 \left(\frac{1}{\varepsilon_A} - \frac{1}{\varepsilon_B}\right)^2 \varepsilon_{0,TM}{}^3 \varepsilon_{0,TE} \left(\frac{\Lambda}{\lambda}\right)^2, \end{aligned} \tag{1}$$

in which f is the grating volume fill factor and ε_A and ε_B are relative permittivities of the grating materials. The zeroth-order permittivity ε_0 in Eq. (1) is given by

$$\varepsilon_{0,TE} = f\varepsilon_A + (1-f)\varepsilon_B \qquad \text{and} \qquad \varepsilon_{0,TM} = \frac{\varepsilon_A \varepsilon_B}{f\varepsilon_B + (1-f)\varepsilon_A} \tag{1}$$

for TE and TM polarization components.

Unfortunately, it is difficult to exactly determine the effective permittivity of a metallic grating based on Eq. (1) and (2) and calculations based on EMT result in large error from measured values since a large negative permittivity of a metal does not produce a converging value for the effective grating permittivity and no such closed-form solutions for a metallic grating has been derived from the EMT[2]. For this reason, the EMT has been applied mainly on dielectric structures. More on that, EMT cannot model lateral shifts of a periodic structure along the direction orthogonal to periodic wires, as complex details of such structure are homogenized through EMT[3]. Addressing these issues can be critical to efficiently analyze metallic periodic structures such as photonic crystals[4,5,6]. In this study, these issues are addressed by a following method: first finding an effective medium of a periodic structure based on effective permittivities obtained from simulating a simple grating structure

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with rigorous coupled wave analysis (RCWA)[7,8] and then fitting the result with a transmittance curve calculated with Fresnel coefficients.

Historically, the most significant disadvantage of using RCWA that in principle is accurate with arbitrary precision over EMT has been that computation based on EMT is much faster than using RCWA. Regarding the advantage of extremely powerful computing capability of present time, however, this is not the case any more. If simple grating structures are considered, calculations of RCWA take oftentimes much less than a few minutes for such configurations. The purpose of this work is therefore to find an effective medium to replace a simple periodic structure based on fitting to RCWA and to finally apply the found effective medium to analyzing more complicated configurations such as photonic crystals.

Consider a simple configuration of tungsten-gratings with a square profile on a silicon substrate, as shown in Fig. 1 (a). The grating period Λ should be small enough in order not to excite higher-order diffraction components. On the other hand, the grating thickness d_g must be large enough not to create surface effects such as surface plasmon resonance or evanescent modes at the top and bottom grating interfaces. In our model, d_g is initially fixed at 1.2 μm and is later altered to check the validity of the acquired effective medium for different grating thickness. The grating period and the fill factor of our model are Λ = 5.4 μm and f = 22% (= 1.2/5.4), respectively. Considering the wavelength of interest in the infrared (λ = 1.5 μm ~ 20 μm), this indicates that the quasi-static condition is not achieved for shorter wavelengths and thus considerable error between the results based on RCWA and EMT is expected. Since higher-order diffraction is incurred at $\lambda = \Lambda/|m|$ normal incidence with m an integer to denote a diffraction order, single-order diffraction prevails for λ > 5.4 μm. If there is such medium as in Fig. 1 (b) which is functionally identical to the grating of Fig. 1 (a), optical characteristics obtained with the grating should fit that of homogenized medium with certain optical indices. We spot those indices by comparing the reflectivity of both configurations by analytically calculating the reflectance of effective medium with Fresnel coefficients.

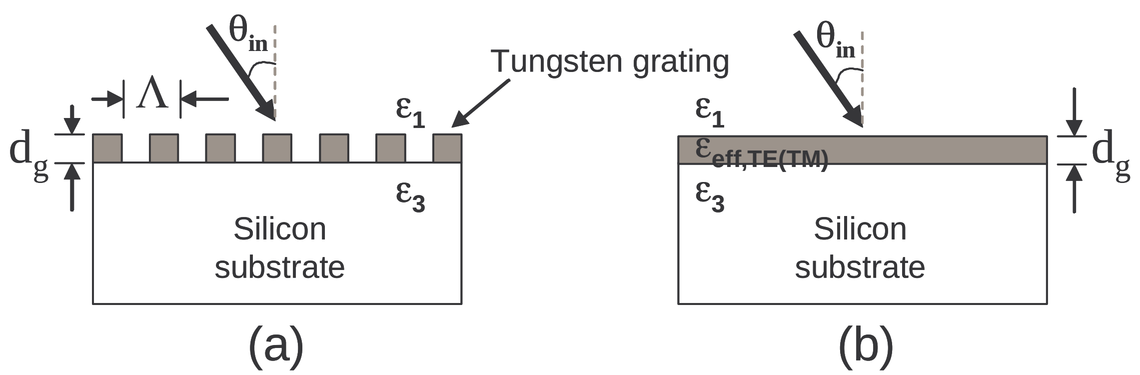

Figure 1 Configurations considered in this paper; (a) a tungsten grating of period Λ and thickness dg is assumed to be deposited on a silicon substrate. (b) An optically equivalent homogeneous anisotropic tungsten film of depth dg is on top of a silicon substrate. A beam is incident at an angle θ_{in}. ε_1 and ε_3 are the permittivity of air and a silicon substrate.

While the calculation of an effective medium is conducted at normal incidence, it should remain valid at an arbitrary incidence angle. This is verified in Fig. 2 which presents the comparison of the reflectance results of TE polarization based on the second-order EMT (dashed) of Eqs. (1) and (2), fitting-based EMT (thick solid) described in this study, and RCWA calculation (thin solid). Figure 2 (a) to (d) corresponds to an incidence angle 0º, 30º, 60º, and 90º. In the shorter wavelength, visible discrepancy is observed, which is expected since the quasi-static condition is not satisfied in this range. Figure 2 shows that when the quasi-static condition is valid, our fitting-based EMT results are in very good agreement with RCWA, compared with the second-order EMT. For TM polarization, the results of which are not shown in this paper, the agreement was generally less robust than TE, which is in line with the results of an earlier study [3].

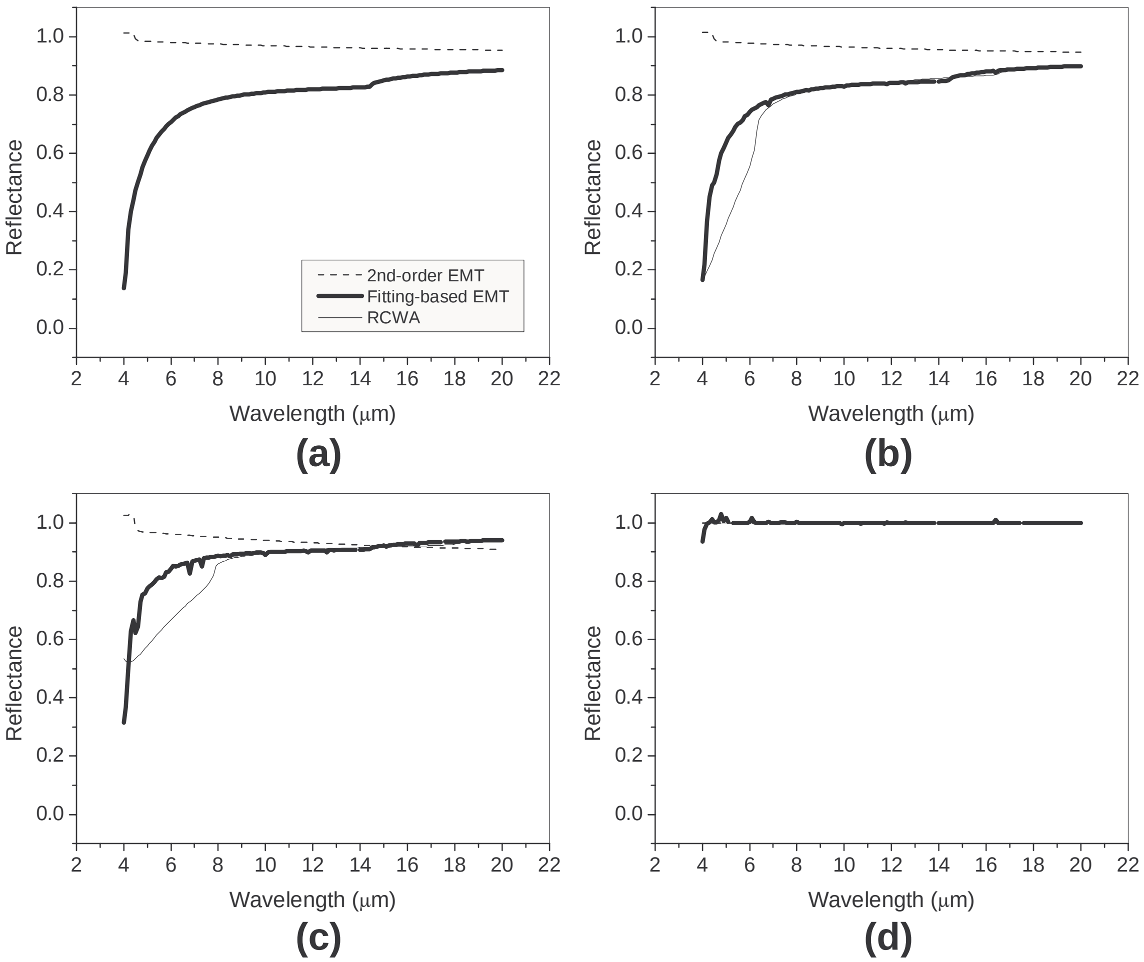

Figure 2 Reflectance of TE polarization when a beam is incident at (a) 0º, (b) 30º, (c) 60º, and (d) 90º. Since the effective permittivities are calculated at normal incidence, fitting-based EMT (thick solid) of (a) shows perfect agreement with RCWA (thin solid), while the second-order EMT (dashed) of Eqs. (1) and (2) shows substantial discrepancy. Fitting-based EMT produces differences from RCWA when the quasi-static condition is not met.

In summary, we have calculated an effective medium of a metallic periodic structure by fitting to RCWA and verified the results for an arbitrary incidence angle. The fitting-based EMT showed general agreement for TE polarization, while the discrepancy is observed for TM. Currently, an improved numerical model is under way to better approximate the TM polarization and furthermore to reproduce optical characteristics of experimental obtained periodic structures.

Acknowledgments

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References

[1] S. M. Rytov, “Electromagnetic properties of a finely stratified medium,” Sov. Phys. JETP **2**, 466-475 (1956).

[2] C. W. Haggans, L. Li, and R. K. Kostuk, “Effective-medium theory of zeroth-order lamellar gratings in conical mounting,” J. Opt. Soc. Am. A **10**, 2217-2225 (1993).

[3] Ph. Lalanne, “Effective medium theory applied to photonic crystals composed of cubic or square cylinders,” Appl. Opt. **35**, 5369-5380 (1996).

[4] J. G. Fleming, S. Y. Lin, I. El-Kady, R. Biswas, and K. M. Ho, “All-metallic three-dimensional photonic crystals with a large infrared bandgap,” Nature **417**, 52-55 (2002).

[5] B. Temelkuran, E. Ozbay, M. Sigalas, G. Tuttle, C. M. Soukoulis, and K. M. Ho, “Reflection properties of metallic photonic crystals,” Appl. Phys. A **66**, 363-365 (1998).

[6] M. M. Sigalas, C. T. Chan, K. M. Ho, and C. M. Soukoulis, “Metallic photonic band-gap materials,” Phys. Rev. B 52, 11744-11751 (1995).

[7] M. G. Moharam and T. K. Gaylord, “Diffraction analysis of dielectric surface-relief gratings,” J. Opt. Soc. Am. **72**, 1385-1392 (1982).

[8] M. G. Moharam and T. K. Gaylord, “Rigorous coupled-wave analysis of metallic surface-relief gratings,” J. Opt. Soc. Am. A **3**, 1780-1787 (1986).