Simulation of micro-mirrors for optical MEMS

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***Abstract*—In this paper we present the application of a computationally efficient Rigorous Coupled-Wave Analysis method to solve the electromagnetic radiation scattering problem in devices featuring nano-structured interfaces and multilayer structures. The method, already successfully used to simulate photon propagation and absorption in thin-film solar cells, is used in this work to compute the optical reflectivity of micro-mirrors in Micro-Opto-Electro-Mechanical Systems (MOEMS).**

***Keywords*—Rigorous Coupled-Wave Analysis (RCWA); Micro-Opto-Electro-Mechanical Systems (MOEMS); optical simulation; electromagnetic solver.**

I. Introduction

The optical scattering of electromagnetic radiation from rough interfaces is a computational problem of interest for several applications involving practical solid-state devices, including optical sensors, solar cells and MOEMS. In such devices, as a consequence of the internal nano-rough interfaces and of the multi-layer scheme featuring layers with thickness significantly smaller or comparable to the radiation wavelength, light scattering is not adequately modeled by simulation methods based on the geometrical optics approximation (e.g. ray tracing) or by methods based on the scalar scattering theory [1] in which the scattering parameters are calibrated by comparison with empirical data. A widely used solver of Maxwell equations suitable for scattering from rough interfaces is that based on the Rigorous Coupled-Wave Method (RCWA) [2]. Differently from standard Transfer Matrix Method (TMM) [3] –whose applicability is essentially limited to flat interfaces- or from algorithms based on the recursive application of the Fresnel equations modified to approximate the effects of the interfacial roughness (for instance IMD simulator [4] or scalar scattering theory exploited by ASA [5]), the proposed enhanced version of Rigorous Coupled-Wave Method (eRCWA) allows simulating arbitrary interface morphologies between layers without limiting the accuracy of the calculations. In addition, calculation by eRCWA is less CPU demanding with respect to other rigorous methods such as the Finite-Difference Time-Domain (FDTD) method [6].

In this paper the optical reflectivity of micro-mirrors for MOEMS fabricated by using several thin protective dielectric films on Aluminum/Silicon based substrates is calculated. This allows to straightforwardly optimize the geometry of visible (VIS) and ultraviolet (UV) mirrors for given dielectric media and substrates by taking into account for process-dependent interface morphologies.

II. Method

In the frame of RCWA, light is modeled as plane waves propagation accounting for optical phenomena occurring in thin-layers such as multiple reflections and interference. RCWA is based on the expansion of the electromagnetic field and of the electromagnetic permittivity in terms of spatial harmonics. In standard RCWA the surface profile is approximated by a set of vertical staircase layers with uniform permittivity. This allows accounting for arbitrary surface morphology, in particular, for the interface random roughness featuring size comparable or even smaller than the radiation wavelength. Within each layer along the vertical axis (Fig. 1, *z*-axis) the wave equation leads to a set of second-order partial differential equations in the Fourier coefficients. This involves the solution of relatively time consuming eigenvalue problem.

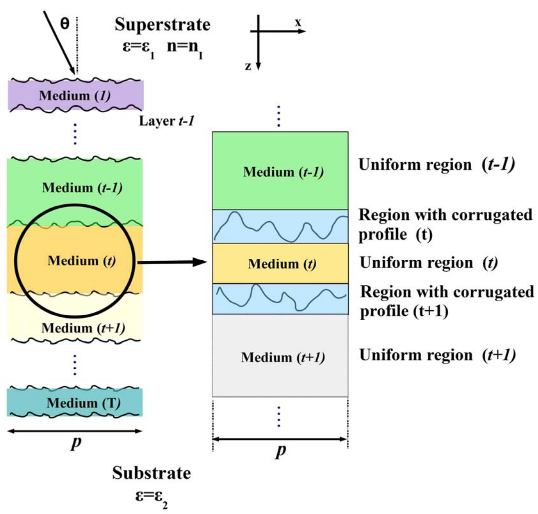

Fig. 1 (left) Two-dimensional (2-D) simulated structure consisting of a multi-layer stack of different materials. Each inter-layer interface exhibits a corrugated profile at the interface between the adjacent one; (right) in eRCWA the structure is divided into uniform regions and into those including the corrugated interfaces (where the permittivity $\varepsilon(x,z)$ is not uniform). $\boldsymbol{\theta}$ denotes the angle of incident radiation with respect to the normal to the device plane and $\boldsymbol{p}$ the periodicity of corrugated profile.

The computational burden of RCWA asymptotically scales as the cube of the total number of harmonics and linearly with the number of staircase layers.

The 2-D eRCWA method used in this work has been introduced in [7], where it was applied to calculate the spatially resolved optical generation rate in thin-film solar cells. Differently from standard RCWA, eRCWA does not solve an eigenvalue problem. Instead, as it will be discussed in the following, eRCWA uses a Dirichlet-to-Neumann map approach within corrugated regions, followed by a differential method to account for nonuniformity along the z-axis. This leads to more computational efficient solver especially in case of thin rough interfaces. However, eRCWA is not particularly efficient when processing deep lamellar gratings where a standard RCWA uses only one staircase layer while eRCWA adopts discretization.

In [7] the proposed simulator has been validated by comparing its accuracy to that of a commercial FDTD program. In [7] the method has been presented with focus on Transverse Electric (TE) light polarization. In this paper we describe the case of TM polarization. In the case of Transverse Magnetic (TM) polarization we must solve the Maxwell equation:

$$\frac{\partial}{\partial z}\left(\frac{1}{\varepsilon(x,z)}\frac{\partial H_y}{\partial z}\right)+\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon(x,z)}\frac{\partial H_y}{\partial x}\right)=-k_0^2 H_y,\ H_x=H_z=0 \quad (1)$$

where $\varepsilon(x,z)$ is the relative permittivity, $k_0^2=\lambda^{-2}(2\pi)^2$ and λ is the wavelength of light. We consider an incident plane-wave propagating in the superstrate region and forming an angle θ with the normal to the device plane (Fig. 1). The device is described as the periodic repetition of a region of finite extension p along the x-axis, with p much larger than the characteristic length of the surface roughness features. Accordingly, we specify the following quasi-periodical Floquet boundary conditions at the boundaries of the simulated element: $H_y(x+p,z)=e^{ik_0 n_I p sin(\theta)}H_y(x,z)$. Such simplifying assumption is reasonable since the thickness of the structure is much smaller than its width and therefore, border effects are negligible. The investigated structure (Fig. 1, left) can be divided into thin regions that include the corrugated profile of the interfaces between media layers and into regions including the uniform portion of layers outside the corrugated region (Fig. 1, right). For each region, we evaluate a S-matrix. In case of a thin interface region ($z_1 \le z \le z_2$, assuming that z_1 and z_2 are the top and bottom boundaries of the corrugated region, respectively) we will search for a solution in the form:

$$H_y(x,z)=\begin{cases}\sum_{s=-N}^{N}\left(c_{1,s}^{+}e^{i\sqrt{k_1^2-k_{xs}^2}(z-z_1)}+c_{1,s}^{-}e^{-i\sqrt{k_1^2-k_{xs}^2}(z-z_1)}\right)e^{ik_{xs}x}, z\le z_1\\ \sum_{s=-N}^{N}\left(d_{1,s}\chi_{1,s}(x,z)+d_{2,s}\chi_{2,s}(x,z)\right), \qquad z_2\le z\le z_1\\ \sum_{s=-N}^{N}\left(c_{2,s}^{+}e^{i\sqrt{k_3^2-k_{xs}^2}(z-z_3)}+c_{2,s}^{-}e^{-i\sqrt{k_2^2-k_{xs}^2}(z-z_2)}\right)e^{ik_{xs}x}, z\ge z_2\end{cases} \quad (2)$$

where $k_l=k_0\sqrt{\varepsilon_l}, l=1,2,\ \ k_{xs}=k_0(n_I sin(\theta)+s\,\lambda/p)$ and n_I is the refractive index of the superstrate. According to equation (2), function $H_y(x,z)$ in the interface region is expanded by means of a set of $M=2N+1$ auxiliary functions $\chi_{j,s}(x,z), j=1,2$ that are required to satisfy equation (1) with the following Dirichlet boundary conditions on top and bottom of the region and the Floquet boundary condition along x-axis:

$$\chi_{1,s}\big|_{z=z_1}=e^{ik_{xs}x},\ \ \chi_{1,s}\Big|_{z=z_2}=0,\ \chi_{2,s}\big|_{z=z_1}=0,\ \ \chi_{2,s}\Big|_{z=z_2}=e^{ik_{xs}x}, \quad (3a)$$

$$\chi_{j,s}(x+p,z)=e^{ik_0 n_I p\sin(\theta)}\chi_{j,s}(x,z) \quad (3b)$$

The auxiliary functions are identified by numerically solving the Dirichlet-like problem given by equations (1), (3a) and (3b) using standard algorithms. In particular, an uniform mesh of N_z nodes is introduced along z-axis within the interface region and functions $\chi_{j,s}(x,z)$ are expanded along x-axis according to a Fourier sum; the number of modes N of the Fourier sum is linked to the number M of auxiliary functions of equation (2): $N=(M-1)/2$. The matrix corresponding to $\varepsilon(x,z)$ is calculated using the inverse rule illustrated in [8]. If we represent the second derivative of H_y with respect to z in equation (1) by means of standard three-point finite-difference scheme, then Fourier coefficients of functions $\chi_{j,s}$ can be determined by means of a block – tridiagonal matrix algorithm (Thomas algorithm). Coefficients c and d are calculated from equation (2) by applying the following matching conditions:

$$H_y\big|_{z=z_i-0}=H_y\big|_{z=z_i+0},\ \frac{1}{\varepsilon(x,z)}\frac{\partial H_y}{\partial z}\bigg|_{z=z_i-0}=\frac{1}{\varepsilon(x,z)}\frac{\partial H_y}{\partial z}\bigg|_{z=z_i+0},\ \ i=1,2 \quad (4)$$

Applying the conditions (3a), (3b) and (4), multiplying the equations by $e^{-ik_{kq}x}$ $(q=-N..N)$, integrating from $x=0$ to $x=p$ and by eliminating coefficients d, we obtain the following equation in S-matrix formulation:

$$\begin{bmatrix}c_2^+\\ c_1^-\end{bmatrix}=S\begin{bmatrix}c_1^+\\ c_2^-\end{bmatrix} \quad (5)$$

where coefficients of the matrix S are combinations of terms:

$$A_{q,s}^{j}=\frac{1}{p}\int_0^p e^{-ik_{xq}x}\frac{\partial\chi_{j,s}(x,z)}{\varepsilon(x,z)\partial z}\bigg|_{z=z_1}dx,\ j=1,2;\ \ q,s=-N..N \quad (6a)$$

$$B_{q,s}^{j}=\frac{1}{p}\int_0^p e^{-ik_{xq}x}\frac{\partial\chi_{j,s}(x,z)}{\varepsilon(x,z)\partial z}\bigg|_{z=z_2}dx,\ j=1,2;\ \ q,s=-N..N\,. \quad (6b)$$

Within the uniform superstrate and substrate regions the field H_y is expressed as the superposition of plane waves:

$$H_y(x,z)=\sum_{s=-N}^{N}\left(c_s^{+}e^{i\sqrt{k_1^2-k_{xs}^2}z}+c_s^{-}e^{-i\sqrt{k_1^2-k_{xs}^2}z}\right)e^{ik_{xs}x}. \quad (7)$$

Thus the S-matrix of the uniform regions featuring thickness Δz is simply a diagonal matrix:

$$\begin{pmatrix}\boldsymbol{c}^+(z+\Delta z)\\ \boldsymbol{c}^-(z)\end{pmatrix}=\mathbf{S}\begin{pmatrix}\boldsymbol{c}^+(z)\\ \boldsymbol{c}^-(z+\Delta z)\end{pmatrix}=\begin{pmatrix}e^{i\sqrt{k_l^2-\boldsymbol{k}_x^2}\Delta z} & 0\\ 0 & e^{i\sqrt{k_l^2-\boldsymbol{k}_x^2}\Delta z}\end{pmatrix}\begin{pmatrix}\boldsymbol{c}^+(z)\\ \boldsymbol{c}^-(z+\Delta z)\end{pmatrix}. \quad (8)$$

By combining the S-matrices of all regions it is possible to obtain the **S**-matrix of the entire structure (Fig.1, left) $\mathbf{s}^{(1,2)}=\mathbf{s}^{(1)}\otimes\mathbf{s}^{(2)}$ which links Fourier coefficients of transmitted and reflected waves with those of the incident wave:

$$\begin{pmatrix}\boldsymbol{c}_{transmitted}\\ \boldsymbol{c}_{reflected}\end{pmatrix}=\boldsymbol{S}\begin{pmatrix}\boldsymbol{c}_{incident}\\ 0\end{pmatrix} \quad (9)$$

III. Results and Discussion

eRCWA is used to calculate the optical properties of an uncoated AlCu mirror starting from its topology as measured by atomic force microscopy (AFM) (Fig. 2, inset). The distribution of surface height is assumed to be described by a Gaussian statistics. Layers thickness, optical constants, surface and interfacial roughness as extracted from spectroscopic ellipsometry (SE), X-ray reflectivity (XRR) and AFM are provided as inputs for the simulator.

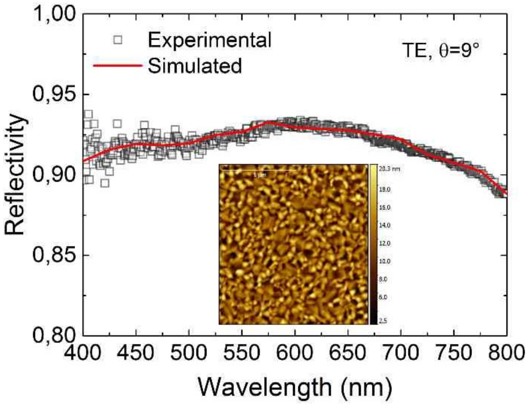

Fig. 2 Measured reflectivity compared to simulated one in the case of an uncoated AlCu mirror (100 nm thick) on Silicon substrate. Transverse Electric (TE) polarization and angle of incidence of light **θ** = 9° are assumed.

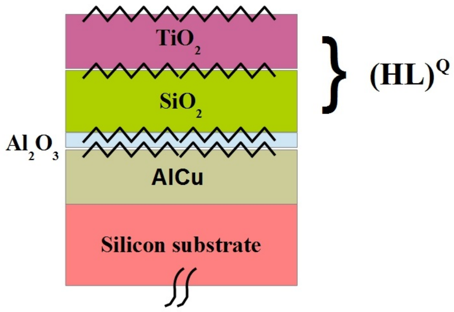

Fig. 3 Sketch of the analyzed coated mirror. An interfacial layer (3 nm Al_2O_3) is assumed between substrate and coating. Roughness is present between AlCu/Si substrate and coating layers as well as at internal interfaces. Coating is a $(HL)^Q$ type, where $\boldsymbol{Q}$ is the periodicity of the HL alternation of high-density and low-density layers.

The eRCWA is applied to the analysis of multi-layer mirrors exhibiting surface roughness determined from AFM maps and assuming rough interfaces among the stacked layers. In our simulation we consider a 10 μm–wide sample and 20000 points are used to describe the interface profile along *x*-axis. As figure of merit, reflectivity characteristics versus radiation wavelength are calculated. In the following, the simulator is employed for the optimization of the thickness of the layers of the mirror protective coatings, based on specifications in terms of reflectivity and spectral response (visible or UV). In particular, we focus on $(HL)^Q$ dielectric mirrors consisting of alternating high and low refractive index layers (Q denotes the periodicity of basic dual-layer stack). In such reflectors (Fig. 3), a stopband window exhibiting enhanced reflectivity can be determined [9, 10]. The stopband window is centered around the design wavelength λ_0. Stopband window width and λ_0 depend on refractive indices of the optically denser and of the less dense layers, n_H and n_L, respectively. By increasing periodicity Q, reflectivity at λ_0 increases, while stopband window shrinks.

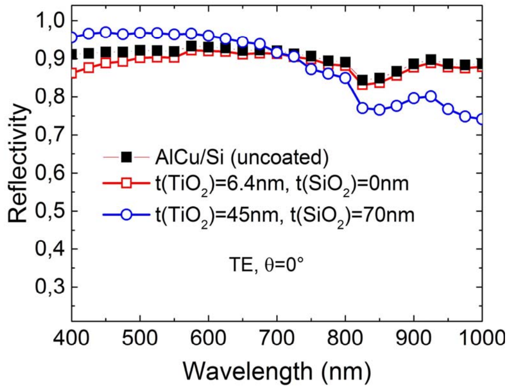

Fig. 4 Calculated reflectivity (TE polarization, normal incidence of light) for uncoated and protected mirrors. Dual-layer reflectivity (Q = 1) compared to that of mono-layer (TiO_2 only). Front interface (Air/TiO_2) is assumed rough with rms value of   = 3 nm.

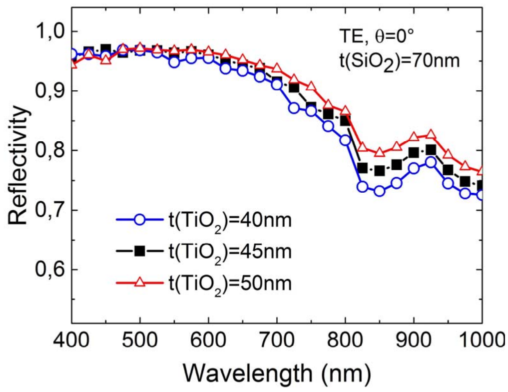

Fig. 5 Calculated reflectivity of TiO_2/SiO_2 coated mirror (Q = 1) for different TiO_2 layer thickness values. Front interface (Air/TiO_2) is assumed rough with rms value of heights σ = 3 nm and correlation length $L = L_0 = 27$ nm.

In order to optimize reflecting surfaces, reflectivity is maximized. In MOEMS an enhanced reflectivity higher than 0.95 for VIS mirrors is a common target. In Fig. 2 simulated reflectivity of a simple uncoated 100 nm-thick AlCu layer on Si substrate is compared to experimental measurements. eRCWA allows to straightforwardly optimize dielectric mirrors in order to attain the enhanced reflectivity condition. As an example of coated AlCu/Si mirror, a TiO_2/SiO_2 (Fig. 3, Q = 1) stack is studied. In our work, at λ = 450 nm n_H = 2.52 and n_L = 1.48, while at λ = 650 nm, n_H = 2.37 and n_L = 1.47. Reflectivity of dielectric mirror is reported and compared to that of an uncoated AlCu surface in Fig. 4. Based on typical experimental results, we assume a rough internal TiO_2/SiO_2 (σ = 3.3 nm, correlation length L = 28 nm).

In addition, exploiting the capabilities of eRCWA, simulation is used to investigate the sensitivity of mirror's optical properties on layer thickness and on interface morphology (Fig. 5 and 6), which are strictly related to fabrication process conditions (choice of deposition precursors, temperature, thermal budget). We observe that increasing roughness leads to reflectivity degradation throughout the spectrum. For roughness σ within a realistic range (σ ≤ 15 nm), reflectivity degradation with respect to an ideally flat surface can reach 5%. Similarly, the sensitivity on layer thickness is significant. A usual design option is based on the number of stacked HL layers Q. Figs. 7 and 8 report the reflectivity of $(HL)^Q$ mirrors tuned for blue and red light sources, respectively. We observe that, to obtain a reflectivity ≥ 0.95 at the design wavelength, Q > 4 is required.

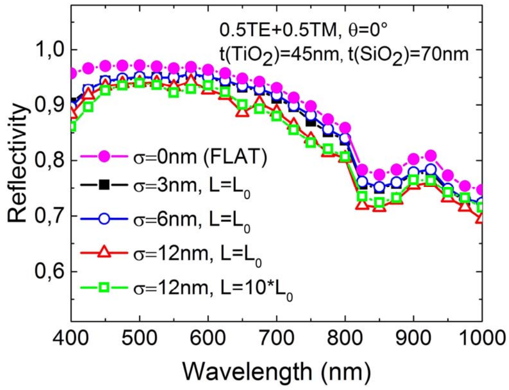

Fig. 6 Sensitivity of reflectivity (simulated) of a dual layer TiO_2/SiO_2 coated mirrors (Q= 1) to front interface roughness   and correlation length L (L_0= 27 nm). Light is unpolarized (50% TE, 50% TM).

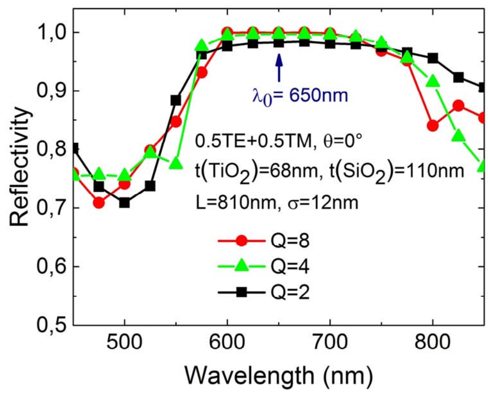

Fig. 7 Calculated reflectivity for AlCu/Si mirrors coated by an alternation of HL TiO_2/SiO_2 stacks with periodicity Q. The coating has been tuned to center the stopband at $\boldsymbol{\lambda_0}$ = 650 nm (red source). External and internal interfaces are rough. Unpolarized light (50% TE, 50% TM) is assumed.

Thanks to the adopted eRCWA tool the typical calculation time on a standard workstation (i.g. dual core Intel Core5 processor with 4 Gb of memory) is 100 seconds per wavelength value. To attain a reasonable accuracy, especially in case of TM polarization (which is more critical for calculation), the number of horizontal modes is typically set to N = 60 and Δz = 1 nm is adopted inside the corrugated region.

IV. CONCLUSIONS

A computationally efficient implementation of RCWA is applied to the calculation of optical reflectivity and to the geometry optimization of mirrors in MOEMS, which are critical components in terms of cost and performance.

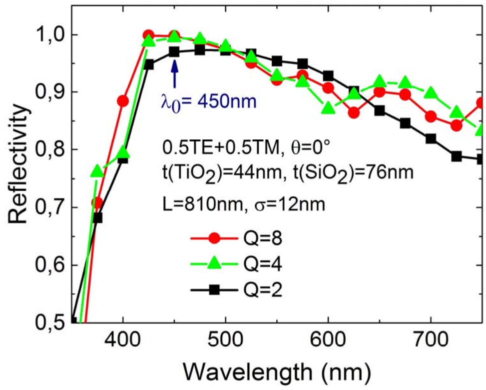

Fig. 8 Calculated reflectivity for AlCu/Si mirrors coated by alternation of TiO_2/SiO_2 stacks with different periodicity Q (2,4 and 8). The HL coating has been tuned to center the stopband at $\boldsymbol{\lambda_0}$ = 450 nm (blue source). External and internal interfaces are rough. Light is unpolarized (50% TE, 50% TM).

Typically, mirrors exhibit multiple thin layers and nanoscale roughness, therefore their design and optimization require an accurate treatment of light scattering. The enhanced version of RCWA here adopted allows to study the sensitivity of the optical properties to process variability and interfaces morphology. Compared to other rigorous numerical solvers of Maxwell equations, eRCWA features similar accuracy and much lower computational cost.

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