Analytic 3D Greens function approach to scattering and diffraction from patterned and/or imperfect multilayers

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ABSTRACT

The 3D electromagnetic Greens function $G_{ij}(\vec{x},\vec{x}')$ for planar multilayers is constructed from the eigenmodes of Maxwell's equations in the multilayer structure. Other approaches have been used to derive the Greens function [1] and the derivation here is similar to that given in [2]. Once obtained this Greens function can be used to perform detailed perturbative calculations of the scattering and diffraction from an arbirtrary nonplanar multilayer in either of two relevant regimes: imperfect or patterned multilayers. For the imperfect case two types of imperfection are considered: mulitiple "point" defects and statistically defined index fluctuations. For patterned multilayers we consider the full structure to built of 2 different basic types of planar structure. Then using the physical optics approximation as the starting or unperturbed field we show that the Greens function easily generates the corrections to this approximation needed to satisfy boundary conditions at the interface between the two planar structure types. Other types of problems can and have been treated by this approach such as mode coupling in linear [3] and nonlinear waveguides [4]. The advantage of using the planar multilayer Greens function follows directly from the fact that it is analytic which provides insight as well as numerical results and the planar eigenmodes can be evaluated rapidly even in 3D so it can be fast.

PLANAR MULTILAYER GREENS FUNCTION

The electromagnetic Greens function for planar multilayer thin films can be constructed using the eigenmodes for planar multilayers. Let x and y be parallel to the multilayers so that z is perpendicular. The multilayers will be indexed with the variable ℓ where $\ell = 0$ corresponds to the substrate, $\ell = 1$ to the first layer on top of the substrate and so on up to $\ell = L$ which is the top layer and $\ell = L + 1$ which is the superstrate (usually taken to be air or vacuum). The z positions of the interfaces between the layers are then given by the list $z_1, z_2, \ldots z_L$ with z_ℓ being the height of the bottom of layer ℓ and hence $z_{\ell+1} - z_\ell$ is the thickness of layer ℓ. Assuming homogeneous isotropic optical properties in each layer, the index of refraction then takes the form $n(z) = n_\ell$ for z in layer ℓ. The two polarization states will be labeled TE and TM. The electric(magnetic) field for the TE(TM) mode has no z component, i.e., it is purely parallel to the interfaces between the layers.

Consider monochromatic fields

$$\begin{aligned}\vec{E}(\vec{x},t) &= e^{-i\omega t}\vec{E}(\vec{x}) \\ \vec{B}(\vec{x},t) &= e^{-i\omega t}\vec{B}(\vec{x})\end{aligned}$$

where $\vec{E}\left(\vec{B}\right)$ is the electric (magnetic) field vector and $\omega = 2\pi f$ is the radian frequency (f is the frequency in Hertz). Then using the "curl E" equation we can represent everything in terms of electric fields, i.e.,

$$\begin{aligned}\vec{E} &= \vec{E}_{TE} + \vec{E}_{TM} \\ &= \vec{E}_{TE} + \left(ic^2/\omega n^2\right)\left(\vec{\partial}\times\vec{B}_{TM}\right)\end{aligned}$$

where c is the speed of light in vacuum and n is the (complex) index of refraction. Expressing everything in terms of $\vec{E}$ Maxwell's equations take the form

$$\left[\left(n^2k^2 + \vec{\partial}^2\right)\delta_{ij} - \partial_i\partial_j\right]E_j = 0 \tag{1}$$

with $k = \omega/c$ and arbitrary $n(\vec{x})$. In regions where the index of refraction n is constant Gauss Law demands $\partial_j E_j = 0$ and the above equation reduces to the standard scalar wave equation. For purely dielectric layers for which $\mathrm{Im}(n) = 0$, taking ∂_i of both sides yields $\vec{\partial}\cdot\left(n^2\vec{E}\right) = 0$ which shows that in this case solutions of the above equation automatically satisfy Gauss Law. The Greens function derived below is for the above operator in the case where $n = n(z)$ can be complex, i.e., for nondielectric planar layers and it satisfies Gauss Law by construction.

For planar multilayers n depends only on z and the x and y dependence can be solved exactly using Fourier transforms. Hence $\vec{E}$ can be written in the form

$$\vec{E}(\vec{\rho},z) = \int d^2\beta e^{i\vec{\beta}\cdot\vec{\rho}}\sum_{p=1}^{3}\xi_p\left(\vec{\beta},z\right)\hat{\varepsilon}_p\left(\vec{\beta}\right) \tag{2}$$

Here $\hat{\varepsilon}_1 = \hat{\beta}\times\hat{z}$, $\hat{\varepsilon}_2 = \hat{\beta}$ and $\hat{\varepsilon}_3 = \hat{z}$ are an orthonormal basis of unit vectors, $\xi_1 = \phi_E$, $\xi_2 = \frac{ic^2}{\omega n^2(z)}\partial_z\phi_M$, $\xi_3 = \frac{c^2\beta}{\omega n^2(z)}\phi_M$, $\beta_x = \vec{k}\cdot\hat{x}$ and $\beta_y = \vec{k}\cdot\hat{y}$ are the x and y

components of the full 3D wave vector $\vec{k}$ and $\vec{\rho} = x\hat{x}+y\hat{y}$. $\phi_E = A_E\phi_E^+ + B_E\phi_E^-$ is a superposition of TE plane wave modes for the planar multilayers with sources at $z = +\infty$ (+superscript)and $z = -\infty$ (−superscript), respectively. ϕ_M is the same but for TM modes. With the above definition $\vec{E}$ satisfies Gauss Law everywhere since it is a superposition of modes which satisfy Gauss Law. In each layer $\phi_E^\pm$ and $\phi_M^\pm$ are linear combinations of upward $(+z)$ and downward $(-z)$ propagating (or evanescent) waves with coefficients chosen to satisfy the TE or TM boundary conditions at each interface. Thus they satisfy

$$\left(n_\ell^2 k^2 - \beta^2 + \partial_z^2\right)\phi_{E,M}^\pm = 0$$

in layer ℓ and the boundary conditions $\phi_E^\pm$ and $\left(\partial_z \phi_E^\pm\right)$ continous at each interface for TE and $\phi_M^\pm$ and $\left(\frac{1}{n^2(z)}\partial_z\phi_M^\pm\right)$ continous at each interface for TM. All these modes have the following explicit form in layer ℓ

$$\begin{aligned}
\phi_\ell^+\left(\vec{\beta}, z\right) &= \frac{T_\ell^+ \exp\left(i\gamma_\ell\left(z_{\ell+1} - z_\ell\right)\right)}{1 - R_\ell^+ R_\ell^- \exp\left(2i\gamma_\ell\left(z_{\ell+1} - z_\ell\right)\right)} \\
&\quad \times \left[\begin{array}{c} R_\ell^- \exp\left(i\gamma_\ell\left(z - z_\ell\right)\right) \\ +\exp\left(-i\gamma_\ell\left(z - z_\ell\right)\right)\end{array}\right] \\
\phi_\ell^-\left(\vec{\beta}, z\right) &= \frac{T_\ell^-}{1 - R_\ell^+ R_\ell^- \exp\left(2i\gamma_\ell\left(z_{\ell+1} - z_\ell\right)\right)} \\
&\quad \times \left[\begin{array}{c} \exp\left(i\gamma_\ell\left(z - z_\ell\right)\right) \\ +R_\ell^+ \exp\left(-i\gamma_\ell\left(z - z_\ell\right)\right)\end{array}\right]
\end{aligned}$$

where $\gamma_\ell = \sqrt{n_\ell^2 k^2 - \vec{\beta}^2}$. For dielectric layers, i.e., $n_\ell =$ real, γ_ℓ is real for $\left|\vec{\beta}\right| < n_\ell k$ and hence the waves are propagating whereas for $\left|\vec{\beta}\right| > n_\ell k$, γ_ℓ is imaginary and the waves are evanescent. For non-dielectric layers, i.e., $n_\ell =$ complex, γ_ℓ is complex for all real values of $\left|\vec{\beta}\right|$ which corresponds to absorption for $\mathrm{Im}\left(n_\ell\right) > 0$ and gain for $\mathrm{Im}\left(n_\ell\right) < 0$. The factor T_ℓ^+ $\left(T_\ell^-\right)$ is the net complex amplitude tranmission factor from the superstrate (substrate) to the top (bottom) of layer ℓ including all the thin film, i.e., multiple reflection, effects in all the bounding layers, and R_ℓ^+ $\left(R_\ell^-\right)$ is the net complex amplitude reflection factor, including all thin film effects, of all the layers above (below) layer ℓ with the phase defined relative to the top (bottom) of the layer. The values of these factors of course depend on the polarization and the value of $\vec{\beta}$. The important point here is that $T_\ell^\pm$ and $R_\ell^\pm$ can easily and rapidly be calculated for TE and TM polarizations using essentially any thin film optics code.

The differential equation defining $G_{ij}\left(\vec{x}, \vec{x}'\right)$ is

$$\delta_{ij}\delta\left(\vec{x} - \vec{x}'\right) = \left[\left(n\left(z\right)^2 k^2 + \vec{\partial}^2\right)\delta_{ik} - \partial_i\partial_k\right] G_{kj}\left(\vec{x}, \vec{x}'\right)$$

where δ_{ij} is a Kronecker delta function and $\delta\left(\vec{x} - \vec{x}'\right) = \delta\left(x - x'\right)\delta\left(y - y'\right)\delta\left(z - z'\right)$, a product of Dirac delta functions. Note that it follows from the above equation that $G_{ij}\left(\vec{x}, \vec{x}'\right)$ has units of inverse length. Letting

$$G_{kj}\left(\vec{x}, \vec{x}'\right) = \frac{1}{\left(2\pi\right)^2}\int d^2\beta e^{i\vec{\beta}\cdot\left(\vec{\rho} - \vec{\rho}'\right)} g_{kj}\left(\vec{\beta}, z, z'\right)$$

and substituting above yields

$$\begin{aligned}
&\delta_{ij}\delta\left(z - z'\right) \\
&= \left[\begin{array}{c} \left(n\left(z\right)^2 k^2 - \beta^2 + \partial_z^2\right)\delta_{ik} \\ +\left(i\beta_i + \delta_{i3}\partial_z\right)\left(i\beta_k + \delta_{k3}\partial_z\right)\end{array}\right] g_{kj}\left(\vec{\beta}, z, z'\right)
\end{aligned}$$

Letting $U = n\left(z\right)^2 k^2$ and rotating to the $\hat{\varepsilon}_p$ basis this reduces to

$$\delta_{pp'}\delta\left(z - z'\right) = \sum_{p''} D_{pp''}\tilde{g}_{p''p'}\left(\vec{\beta}, z, z'\right)$$

with

$$D_{pp''} = \left[\begin{array}{ccc} U - \beta^2 + \partial_z^2 & 0 & 0 \\ 0 & U + \partial_z^2 & -i\beta\partial_z \\ 0 & -i\beta\partial_z & U - \beta^2 \end{array}\right]$$

The solution is given by

$$\begin{aligned}
\tilde{g}_{pp'} &= \frac{1}{N_{p'}\left(\vec{\beta}, z'\right)}\left[\begin{array}{c} \theta\left(z - z'\right)\xi_p^-\left(\vec{\beta}, z\right)\xi_{p'}^+\left(\vec{\beta}, z'\right) \\ +\theta\left(z' - z\right)\xi_p^+\left(\vec{\beta}, z\right)\xi_{p'}^-\left(\vec{\beta}, z'\right)\end{array}\right] \\
&\quad + \frac{\delta_{p3}\delta_{p'3}}{U}\delta\left(z - z'\right)
\end{aligned}$$

for $(p, p') = (1, 1), (2, 3), (3, 2)$ and $(3, 3)$ and is zero otherwise. The Normalization factors, $N_{p'}\left(\vec{\beta}, z'\right)$ are essentially Wronskian functions and are given by

$$\begin{aligned}
N_1\left(\vec{\beta}, z\right) &= \left(\partial_z\xi_1^-\right)\xi_1^+ - \left(\partial_z\xi_1^+\right)\xi_1^- \\
N_2\left(\vec{\beta}, z\right) &= \left(\partial_z\xi_2^-\right)\xi_2^+ - \left(\partial_z\xi_2^+\right)\xi_2^- \\
&\quad - i\beta\left(\xi_3^-\xi_2^+ - \xi_3^+\xi_2^-\right) \\
N_3\left(\vec{\beta}, z\right) &= i\frac{U}{\beta}\left(\xi_3^-\xi_2^+ - \xi_3^+\xi_2^-\right)
\end{aligned}$$

The delta function in $\tilde{g}_{33}$ is a standard singularity that occurs in TM boundary conditions [2] and is required to make $\left(D\tilde{g}\right)_{23} = 0$. This result can be written in an arbitrary x, y, z coordinate system with $\hat{e}_i$, $i = x, y, z$ unit vectors using

$$g_{ij} = \sum_{pp'}\tilde{g}_{pp'}\left(\hat{\varepsilon}_p\cdot\hat{e}_i\right)\left(\hat{\varepsilon}_{p'}\cdot\hat{e}_j\right)$$

Note finally that since $G_{ij}\left(\vec{x}, \vec{x}'\right)$ is constructed as a superposition of eigenmodes of the multilayer it automatically includes all nominal thin film diffraction effects.

SCATTERING AND DIFFRACTION FROM NONPLANAR LAYERS

For a generic nonplanar multilayer structure, i.e., a patterned or imperfect multilayer, the wave equation, Eq(1), is as given above but with $n = n(\vec{x})$. Writing the difference in the square of the index between the actual case and the "closest" planar multilayer in the form $n(\vec{x})^2 = n(z)^2 - \eta(\vec{x})$ where the minus sign is for later convenience and letting $\vec{E} = \vec{E}^0 + \vec{E}^S$ where $\vec{E}^0$ is the electric field solution for the planar structure and $\vec{E}^S$ is the "excess" scattering/diffraction caused by the difference between the real structure and the planar structure, substituting in the wave equation and finally using the fact that $\vec{E}^0$ satisfies the planar structure wave equation we get

$$\left[\left(n(z)^2 k^2 + \vec{\partial}^2\right)\delta_{ij} - \partial_i\partial_j\right] E_j^S = \eta(\vec{x})\, k^2 \left(E_j^0 + E_j^S\right)$$

Using the Greens function developed in the previous section we can rewrite this as the integral equation

$$\begin{aligned} E_i^S(\vec{x}) &= k^2 \sum_j \int d^3x' G_{ij}(\vec{x},\vec{x}')\, \eta(\vec{x}')\, E_j^0(\vec{x}') \\ &\quad + k^2 \sum_j \int d^3x' G_{ij}(\vec{x},\vec{x}')\, \eta(\vec{x}')\, E_j^S(\vec{x}') \end{aligned}$$

This has the form of a Schwinger-Dyson equation for $E_i^S(\vec{x})$. Iterating yields the series solution

$$E_i^S(\vec{x}) = \sum_{q=1}^{\infty} k^{2q} \int d^3x' \,(G\eta)_{ij}^q (\vec{x},\vec{x}')\, E_j^0(\vec{x}')$$

where $(G\eta)^q$ is understood to contain the appropriate combination of matrix multiplication and integration for each value of q. The total electric field is given by simply including the $q = 0$ term in the summation

$$\begin{aligned} E_i(\vec{x}) &= E_i^0(\vec{x}) + E_i^S(\vec{x}) \\ &= \sum_{q=0}^{\infty} k^{2q} \int d^3x' \,(G\eta)_{ij}^q (\vec{x},\vec{x}')\, E_j^0(\vec{x}') \end{aligned}$$

Below this formalism is applied to determining the contribution to the electric field caused by various deviations from pure planarity of the multilayer. Space limitations severely restrict the extent and depth of the discussion and so detailed analysis of a broad range of specific cases will have to await publication elsewhere. Also, only the lowest order contributions are considered.

Imperfect Layers

Many types of imperfections can and do occur in planar multilayers. The two basic types considered here are multiple localized index deviations and statistically defined fluctuations $\eta(\vec{x})$.

Index deviations that are highly localized, i.e., are much smaller than the wavelength in the region where the deviation occurs, can be treated as essentially point sources which eliminates the integrations. That is we can write

$$\eta(\vec{x}) = \sum_m V_m \eta_m \delta(\vec{x} - \vec{x}_m)$$

where V_m is the volume of the index deviation η_m located at $\vec{x}_m$. Then $E_i^S(\vec{x})$ is given by

$$E_i^S(\vec{x}) = k^2 \sum_m G_{ij}(\vec{x},\vec{x}_m)\, V_m \eta_m E_j^0(\vec{x}') + \cdots$$

As might be expected this is the single scattering case and the higher order terms progressively account for double, triple, etc. scattering. Although this result is rather obvious it must be remembered that all the nominal thin film diffraction effects are automatically included.

Zero mean, $\langle \eta(\vec{x}) \rangle = 0$, statistical index fluctuations can be defined by the autocorrelation function

$$\langle \eta(\vec{x})\, \eta^*(\vec{x}') \rangle = C(\vec{x},\vec{x}')$$

Additionally, if we assume translationally invariant statistics then $C(\vec{x},\vec{x}')$ can be replaced with $C(\vec{x}-\vec{x}')$. This is the case considered here. The autocorrelation function of the scattered electric field is then given simply by

$$\begin{aligned} &\left\langle E_i^S(\vec{x})\, E_j^{S*}(\vec{x}') \right\rangle \\ &= k^4 \sum_{kl} \int d^3x_1 d^3x_2 \left[\begin{array}{c} G_{ik}(\vec{x},\vec{x}_1)\, G_{jl}^*(\vec{x}',\vec{x}_2) \\ \times E_k^0(\vec{x}_1)\, E_l^{0*}(\vec{x}_2)\, C(\vec{x}_1 - \vec{x}_2) \end{array} \right] \\ &\quad + \cdots \end{aligned}$$

Setting $\vec{x} = \vec{x}'$ and summing over $i = j$ yields the expectation of the scattered intensity again including all nominal thin film effects.

Patterned Layers

Lithographic masks or reticles can be transmissive or reflective. Both binary and phase shift masks can be viewed as being built up of several discrete different planar layer structures. Here we consider two different planar structures labeled a and b, with index distributions $n_a(z)$ and $n_b(z)$, respectively. Both structures are defined over the same z range z_{bot} to z_{top} but the value of the index at any given z will in general be different between the two. Let $S_a(\vec{x}) = S_a(\vec{\rho}, z) = 1$ for $\vec{\rho}$ in structure a and similarly define $S_b(\vec{\rho}, z)$. The physical optics "solution" to this problem can be written in the form

$$E_i^{po}(\vec{x}) = \begin{cases} S_a(\vec{x})\, E_i^a(\vec{x}) + S_b(\vec{x})\, E_i^b(\vec{x}) \\ \text{for } z_{bot} < z < z_{top} \\ E_i^{in+}(\vec{x}) + E_i^{refl+}(\vec{x}) + E_i^{tran+}(\vec{x}) \\ \text{for } z > z_{top} \\ E_i^{in-}(\vec{x}) + E_i^{refl-}(\vec{x}) + E_i^{tran-}(\vec{x}) \\ \text{for } z < z_{bot} \end{cases}$$

Here $\vec{E}^{in\pm}$ is the incoming field from $z = \pm\infty$ and $\vec{E}^{relf\pm}$ and $\vec{E}^{tran\pm}$ are the physical optics approximation net reflected and transmitted fields, respectively, from the structured multilayer in the regions above and below the structure. These are generated by propagating the reflected and transmitted fields from planes just above and below the structure to the desired position. This propagation can be done most simply using Fourier transforms. For example if the reflected field at the plane $z = z_{top}$ is represented as

$$E_i^{refl+}(\vec{\rho}, z = z_{top}) = \int d^2\beta e^{i\vec{\beta}\cdot\vec{\rho}} \tilde{E}_i^{refl+}\left(\vec{\beta}\right)$$

then the propagated field is given by

$$E_i^{refl+}(\vec{\rho}, z > z_{top}) = \int d^2\beta e^{i\vec{\beta}\cdot\vec{\rho}+i\gamma(z-z_{top})} \tilde{E}_i^{refl+}\left(\vec{\beta}\right)$$

where $\gamma = \sqrt{k^2 - \beta^2}$. The function $\tilde{E}_i^{refl}\left(\vec{\beta}\right)$ is easily determined using the mode expansion given in Eq(2).

Subsituting $\vec{E} = \vec{E}^{po} + \vec{E}^S$ into Eq(1) will generate terms involving derivatives of the S functions as well as S times the wave equation operating on $\vec{E}^{po}$ which vanishes by construction. Since the S functions are discontinuous at the interfaces or boundaries between structures a and b their derivatives yield Dirac delta functions and derivatives of Dirac delta functions with arguments that vanish on these interfaces. Hence these terms act as "boundary" sources for $\vec{E}^S$ and their effect is to generate the corrections to $\vec{E}^{po}$ required to satisfy the standard boundary conditions on these interfaces. Their values are essentially given by the discontinuity in $\vec{E}^{po}$ and its derivatives across the boundary. If these terms vanished as well then $\vec{E}^{po}$ would be the exact correct solution including boundary conditions. Writing this "boundary" term generically in the form $\hat{B}E_i^{po}$ and noting that

$$n(\vec{x})^2 = S_a(\vec{x})\, n_a(z)^2 + S_b(\vec{x})\, n_b(z)^2$$

the wave equation becomes

$$\left[\begin{array}{c} \left(S_a(\vec{x})\, n_a(z)^2 + S_b(\vec{x})\, n_b(z)^2\right) k^2\delta_{ij} \\ +\vec{\partial}^2\delta_{ij} - \partial_i\partial_j \end{array}\right] E_j^S = \hat{B}E_i^{po}$$

which can be solved using Greens function for either the a or b structure or for some average of the two. To be specific we use the a structure Greens function, G_{ij}^a with the result

$$\begin{aligned} E_i^S &= \sum_j \int d^3x' G_{ij}^a(\vec{x}, \vec{x}') \\ &\times \left(\begin{array}{c} \left(\hat{B}E_i^{po}\right)(\vec{x}') \\ +k^2 S_b(\vec{x}')\left(n_a(z)^2 - n_b(z)^2\right) E_i^S(\vec{x}') \end{array}\right) \end{aligned}$$

The lowest order term is the direct correction to the electric assumed physical optics solution due the deviation of $\vec{E}^{po}$ from required boundary conditions at the ab interfaces. The higher order terms come from the propagation of these corrections between interfaces and the consequent readjustment of the field discontinuities there.

It should be noted that although we have treated discrete step discontinuities in the structure the same generic approach can be used for slowly varying index deviations such as a multilayer thin film coating conforming to a bump or divot in the substrate.

CONCLUSIONS

The derivation of the Greens function for planar multilayers has been discussed along with its application to several generic problems dealing with scattering and diffraction from nonplanar multilayers. The Greens function is represented analytically as a superposition of thin film modes and thus its evaluation is straightforward and can be done rapidly using essentially any thin film optics code. Athough this technique has seen its greatest application in the area of coupled mode analysis of waveguides it clearly can be applied to studying the scattering and diffraction from lithographic masks and reticles. In particular it can be applied to EUV lithography masks to determine the diffracted field for a given pattern and to determine the effect of defects in the multilayers on image quality.

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