S-matrix approach for calculations of the optical properties of metallic-dielectric photonic crystal slabs

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Photonic crystal slabs (PCS)

Layers may be composed of dielectrics, metals, semiconductors

Peculiarities in optical spectra

- Diffractive
  - (opening of diffractive channels as $\lambda$ decreases)

- Waveguide

- Plasmonic Resonances
  - (localized and delocalized)
Transfer-matrix method

Transfer matrix combines the amplitudes at different planes $a$ and $b$

\[
\begin{pmatrix}
\vec{A}_a^+ \\
\vec{A}_b^-
\end{pmatrix}
\begin{pmatrix}
\vec{A}_b^+ \\
\vec{A}_a^-
\end{pmatrix}
= T_{a,b}
\begin{pmatrix}
\vec{A}_a^+ \\
\vec{A}_b^-
\end{pmatrix}
\]

Scheme of calculations

1) Splitting of the structure into layers along Oz
2) Floquet-Fourier expansion of the Maxwell's equations in each layer
3) Calculation of transfer, interface and total transfer matrices through the structure
4) Calculation of transmission, reflection, absorption

T-matrix is numerically instable for PCSs (mixing of exponentially increasing and decreasing modes)
Scattering-matrix method

S-matrix combines the input amplitudes with the output ones

\[
\begin{pmatrix}
A_+^a \\
A_-^a \\
A_+^b \\
A_-^b
\end{pmatrix}
= \mathbf{S}_{a,b}
\begin{pmatrix}
A_+^a \\
A_-^a \\
A_+^b \\
A_-^b
\end{pmatrix}
\]

Scheme of calculations

1) Splitting of the structure into layers along Oz
2) Floquet-Fourier expansion of the Maxwell's equations in each layer
3) Calculation of the transfer matrix for field amplitudes
4) Iterative calculation of the scattering matrix, Ko&Inkson (1988)
5) Calculation of transmission, reflection, absorption and diffraction

—Whittaker&Culshaw, PRB 60, 2610 (1999)
Scattering matrix approach

Advantages of the method:
1) No additional fitting parameters, only structure's geometry and epsilon data
2) Calculation of the near-field distribution
3) All calculation can be performed on PC

Limitations of the method:
1) Slow convergence for metallic-dielectric layers
2) Time of calculations $\sim N_g^3$, $N_g$ - number of used harmonics

Additions to the method$^1$: adaptive spatial resolution$^2$

Improved convergence$^1$!!!

Accuracy of the solution (eigenvalues)$^2$???

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Accuracy of the eigenvalue calculations

Compare two calculation schemes

- **S-matrix** (factorization rules)
- **S-matrix improved** (with adaptive spatial resolution and factorization rules)

Eigenvalues in the periodic layer \( K(n) = K(n)(k_{x_0}, \omega) \)

\( n=1, \ldots, 2N_g, N_g \) - number of used harmonics

It is not possible to check the accuracy of \( K \) directly!

Using T-matrix over the period and some math...

\[
T_d = T_{d_2} T_{2 \rightarrow 1} T_{d_1} T_{1 \rightarrow 2} \Rightarrow k_x^{(n)} = k_x^{(n)}(K(n), \omega)
\]

\[
k_{x_0} = \frac{\omega}{c} \cos \theta
\]

- compare two values

Gold nanowires on top of quartz substrate
Accuracy of the eigenvalue calculation

\[ k_x^{(n)} = k_x^{(n)}(K^{(n)}, \omega) \]
\[ k_{x0} = \frac{\omega}{c} \cos \theta \]

\[
\lim_{N_g \to \infty} \ln \left( \frac{|k_x^{(n)} - k_{x0}|}{k_{x0}} \right) = -\infty \quad \text{n=const (fixed harmonic)}
\]

**TE - polarization**

Energy=1200 meV, \( K_{x0} = 4.3 \, \mu m^{-1} \), \( \varepsilon_1 = -45.2 + 3.26i \), \( \varepsilon_2 = 1 \)

- improved S-matrix
- S-matrix

**TM - polarization**

Energy=1200 meV, \( K_{x0} = 4.3 \, \mu m^{-1} \), \( \varepsilon_1 = -45.2 + 3.26i \), \( \varepsilon_2 = 1 \)

- improved S-matrix
- S-matrix
S-matrix calculations of the optical properties

dispersion relation of the waveguide modes

\[ \det(S^{-1}(\omega, k_{\parallel})) = 0 \]

Air light cone
Substrate light cone
Waveguide light cone

L_z = 300 nm; \( \varepsilon_1 = 1; \varepsilon_2 = 4; \varepsilon_3 = 2.13 \)
S-matrix calculations of the optical properties

dispersion relation of the surface plasmon polariton

\[ \det(S^{-1}(\omega, k_||)) = 0 \]

\( \varepsilon_{Ag} \) – calculated using Lorentz-Drude model

\[ \varepsilon_1 = 1; \ varepsilon_2 = Ag; \ varepsilon_3 = 2.13 \]

\[ L_z = 50 \text{ nm} \]
\[ L_z = 30 \text{ nm} \]
\[ L_z = 10 \text{ nm} \]

Air light cone
Substrate light cone

\(^1\text{A. D. Rakić et al., Applied Optics, Vol. 37, No. 22 (1998)}\)
S-matrix calculations of the optical properties

1) Localized plasmon in gold nanowires (Energy~1.8 eV)

2) Delocalized plasmon in the silver film (excitation due to periodic corrugation)

3) Interaction of the resonances

Structure parameters:

\[ w_{Au} = 100 \text{ nm}, \ h_{wire} = 20 \text{ nm}, \ L_z = 40 \text{ nm}, \ h_{film} = 10 \text{ nm}, \ d_x = 200-350 \text{ nm} \]
S-matrix calculations of the optical properties

Structure parameters:
\( w_{\text{Au}} = 100 \text{ nm}, h_{\text{wire}} = 20 \text{ nm}, L_{\text{z}} = 40 \text{ nm}, h_{\text{film}} = 10 \text{ nm}, d_{\text{x}} = 200-350 \text{ nm} \)

Period = 200 nm

Dispersion relation of bare plasmon modes

Calculated extinction spectrum

Normal light incidence, TM - polarization
S-matrix calculations of the optical properties

Structure parameters:
$w_{Au} = 100 \text{ nm}$, $h_{wire} = 20 \text{ nm}$, $L_z = 40 \text{ nm}$, $h_{film} = 10 \text{ nm}$, $d_x = 200-350 \text{ nm}$

Period = 350 nm

Dispersion relation of bare plasmon modes

Calculated extinction spectrum

Normal light incidence, TM - polarization
S-matrix calculations of the optical properties

Near-field distribution at resonances

Electric field

Magnetic field

Field Energy 1220 meV
S-matrix calculations of the optical properties

Near-field distribution at resonances

Electric field

Magnetic field
Conclusions

1) Scattering matrix approach is a powerful tool for calculations of the PCS

1) Accuracy of the two calculation schemes were compared. Improved scheme shows better results for TM polarization and not large number of harmonics < 121

1) Extinction spectra and near-field distribution of the specific structure have been modeled theoretically
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Thank you for your attention!