Inverse design of resonant nanostructures for extraordinary optical transmission of periodic metallic slits

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Abstract

This paper presents the inverse design of resonant nanostructures for the extraordinary optical transmission of periodic metallic slits, where the topology optimization approach is utilized to implement the inverse design procedure and find the geometrical configurations of the nanostructures. By the inverse design method, the subwavelength-size resonant nanostructures, localized at the inlet and outlet sides of the periodic metallic slits, are derived with transmission peaks at the prescribed incident wavelengths. And the transmissivity is enhanced by effective excitation and guidance of surface plasmon polariton at the inlet side of the slits, coherently resonance of surface plasmon polariton inside the slits and radiation of the photonic energy at the outlet side of the slits. The transmission peaks of the periodic metallic slits, with inversely designed resonant nanostructures, are raised along with the red shift of the incident wavelength. The presentation of the transmission peak of periodic metallic slits can be controlled and localized at a desired frequency, by specifying the incident wave with the wavelength corresponding to the desired frequency for the inverse design procedure. By maximizing the minimum transmissivity of the periodic metallic slits with incident wavelengths in a prescribed wavelength range, the extraordinary optical transmission bandwidth can be enlarged, and the sensitivity of transmissivity to wavelength can be decreased equivalently.

Keywords: Inverse design; resonant nanostructures; extraordinary optical transmission; periodic metallic slits; topology optimization

1 Introduction

Extraordinary optical transmission (EOT) is the phenomenon of greatly enhanced transmission of light through a subwavelength aperture in an otherwise opaque metallic film which has been patterned with a regularly repeating periodic structure. It was first described by Ebbesen et al in 1998 [1]. In EOT, the regularly repeating structures enable much higher transmissivity to occur, up to several orders of magnitude greater than that predicted by classical aperture theory. And the mechanism of EOT is attributed to the scattering of surface plasmon polaritons (SPPs) [2,3]. EOT offers one key advantage over a surface plasmonic resonance (SPR) device, an inherently nanometer-micrometer scale device, and it is particularly amenable to miniaturization. Tremendous potential applications of EOT include several newly emerging areas, e.g.

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subwavelength optics, opto-electronic devices, wavelength-tunable filters, optical modula-
tors [5,6], left-handed metamaterial and chemical sensing [7]. To achieve the required
transmission performance, metallic layouts with subwavelength apertures, e.g. subwave-
length hole array [1], periodic slit array, tapered slits [8], diatomic chain of slit-hole [9],
groove array flanking slit [10] and bull’s eye structures [11], have been proposed for
EOT; and parametric optimization of metallic layouts with subwavelength apertures
have been implemented to enhance the transmissivity [12,13]. Most of these researches
are focused on enhancing EOT with nanostructures derived based on physical intuition.
The more challenging problem problem can be inverse design or determination of the
geometrical configurations of the nanostructures for enhancing EOT. Therefore, this
paper is devoted to inversely designing resonant nanostructures to enhance the extraor-
dinary optical transmission of periodic metallic slits, where the topology optimization
approach is utilized to implement the inverse design method and find the geometrical
configurations of the nanostructures.

Recently, it is shown that topology optimization can be used to inversely deter-
mine geometrical configuration of structures and achieve the inverse design of devices
in elastics, hydrodynamics, electromagnetics or photonics et al [14,17]. In electromag-
netics or photonics, topology optimization approach has been applied in the inverse
design of beamsplitters [18,19], photonic crystals [20,22], cloaks [23,25], metamate-
rials [26,28], excitation of SPPs and LSPRs [29,30], and electromagnetic and optical
antennas [31,34]. In topology optimization, the structure is inversely determined using
the material penalization approach, where the design variable is used to represent the
material distribution and geometrical configuration. The design variable is evolved to
a indicator function using the robust gradient based optimization algorithm, e.g. the
method of moving asymptotes (MMA) [35]. Therefore, the topology optimization ap-
proach is chosen to implement the inverse design of the nanostructures of the periodic
metallic slits for EOT.

2 Methodology

Cross-section of periodic metallic slits with infinite thickness is illuminated in Fig. 1
with a uniform monochromatic transverse magnetic (TM) wave propagation. The com-
putational domain is set to be one period of the metallic slits. The topology optimization
approach is utilized to inversely design the nanostructures localized in the bilateral re-
gions of the preset metallic slits. Then the design domain, where the design variable is
defined, is set to be these two bilateral regions. To truncate the infinitive free space,
the first order absorbing boundary condition is imposed on the inlet (Γ1) and outlet
(Γo) boundaries of the computational domain, and the periodic boundary condition is
imposed on the left (Γps) and right (Γpd) boundaries of the slit to reduce the computa-
tional cost. Based on the above computational setup, the inverse design problem is to
find the geometrical configurations of the bilateral nanostructures for the preset slit to
maximize the transmission of the electromagnetic energy. The propagating wave in the
metallic slits is time-harmonic TM wave governed by the Maxwell’s equations in two
dimensions, which can be reformulated into the scalar Helmholtz equation expressed as

\[ \nabla \cdot \left[ \epsilon_r^{-1} \nabla (H_{zs} + H_{z1}) \right] + k_0^2 \mu_r (H_{zs} + H_{z1}) = 0, \quad \text{in } \Omega \]

\[ \epsilon_r^{-1} \nabla H_{zs} \cdot \mathbf{n} + jk_0 \sqrt{\epsilon_r^{-1} \mu_r} H_{zs} = 0, \quad \text{on } \Gamma_1 \cup \Gamma_o \]

\[ H_{zs}(\mathbf{x} + \mathbf{a}) = H_{zs}(\mathbf{x}) e^{-jk \cdot \mathbf{a}}, \quad \mathbf{n}(\mathbf{x} + \mathbf{a}) \cdot \nabla H_{zs}(\mathbf{x} + \mathbf{a}) = -e^{-jk \cdot \mathbf{a}} \mathbf{n}(\mathbf{x}) \cdot \nabla H_{zs}(\mathbf{x}), \quad \text{for } \forall \mathbf{x} \in \Gamma_{ps}, \ \mathbf{x} + \mathbf{a} \in \Gamma_{pd} \]

where the scattered-field formulation, with \( H_z = H_{zs} + H_{z1} \), is used to reduce the
dispersion error; \( H_{zs} \) and \( H_{z1} \) are the scattered and incident fields, respectively; \( \epsilon_r \) and
\( \mu_r \) are the relative permittivity and permeability, respectively; \( k_0 = \omega \sqrt{\epsilon_0 \mu_0} \) is the free
space wave number with \( \omega, \epsilon_0 \) and \( \mu_0 \) respectively representing the angular frequen-
cy, free space permittivity and permeability; \( \Omega \) is the computational domain; \( \mathbf{k} \) is the wave
vector; the time dependence of the fields is given by the factor \( e^{j \omega t} \), with \( t \) representing
the time; \( \mathbf{n} \) is the unit outward normal vector at \( \partial \Omega \); \( j = \sqrt{-1} \) is the imaginary unit; \( \Gamma_1 \)
and \( \Gamma_o \) are respectively the inlet and outlet boundaries of the photonic energy; and \( \Gamma_{ps} \)
and $\Gamma_{pd}$ are respectively the source and destination boundary of the periodic boundary pair, with lattice vector $\mathbf{a}$. The incident field $\mathbf{H}_z$ is set to be the parallel-plane wave with unit amplitude.

![Diagram](image)

**Figure 1**: Computational domain for the inverse design of bilateral nanostructures for the periodic metallic slits, where $\mathbf{H}_z$ is the propagating TM wave; $\mathbf{k}$ is the wave vector; $\Omega_f$, $\Omega_d$ and $\Omega_m$ are the free space, design and metallic domains, respectively; $\Gamma_i$ and $\Gamma_o$ are inlet and outlet boundaries of the photonic energy, respectively; $\epsilon_{rf}$, $\epsilon_{rd}$ and $\epsilon_{rm}$ respectively are the relative permittivity in $\Omega_f$, $\Omega_d$ and $\Omega_m$; $\Gamma_{ps}$ and $\Gamma_{pd}$ are the source and destination boundary of the periodic boundary pair, respectively; $\Omega = \Omega_f \cup \Omega_d \cup \Omega_m$ is the computational domain.

The topology optimization approach, chosen to carry out inverse design of bilateral nanostructures for enhancing EOT of periodic metallic slits, is implemented based on the material interpolation between the metal and free space in the design domain. In EOT, the used noble metal is usually nonmagnetic, e.g. silver (Ag) and gold (Au). Therefore, the permeability is set to be 1. Then, only the spatial distribution of relative permittivity needs to be determined in the inverse design procedure. In the visible light region, the relative permittivity of noble metal can be described by the Drude model

$$\epsilon_{rm} = \epsilon_{r\infty} - \frac{\omega_p^2}{\omega (\omega - j\gamma_c)} \quad (2)$$

where $\epsilon_{r\infty}$ is the high-frequency bulk permittivity; $\omega$ is the angular frequency of the incident wave; $\omega_p$ is the bulk plasmon frequency; $\gamma_c$ is the collision frequency. The material interpolation is performed using the material density representing the geometrical configuration [39], and the material density is introduced with the values 0 and 1 respectively representing free space and metal. Because the surface plasmons are presented at the surface of noble metal, the electromagnetic field decays exponentially; hence, the material density should decays rapidly away from 1 to mimic the metal surface. Thus, the material interpolation is set to be the hybrid of logarithmic and power law approaches

$$\epsilon_{rd}(\omega) = 10^{\log \epsilon_{rm}(\omega) - \frac{-1}{1+\bar{\rho}^3} [\log \epsilon_{rm}(\omega) - \log \epsilon_{rf}(\omega)] \tanh (\beta \xi) + \tanh (\beta (\bar{\rho} - \xi)) \tanh (\beta \xi) + \tanh (\beta (1 - \xi))} \quad (3)$$

where $\epsilon_{rd}$ is the relative permittivity in the design domain; $\bar{\rho}$ is the material density. The material density is derived by filtering and projecting the design variable valued in $[0, 1]$. During the evolution of the design variable, filtering is implemented by the density filter to enforce a minimum length scale of the derived geometrical configuration

$$-r^2 \nabla \cdot \nabla \bar{\rho} + \bar{\rho} = \rho, \text{ in } \Omega$$

$$\nabla \bar{\rho} \cdot \mathbf{n} = 0, \text{ on } \partial \Omega \quad (4)$$

where $r$ is the filter radius chosen based on numerical experiments [37]; $\bar{\rho}$ is the filtered design variable. And projecting is implemented by the threshold projection to remove the gray area in the derived geometrical configuration [38]

$$\bar{\rho} = \frac{\tanh (\beta \xi) + \tanh (\beta (\bar{\rho} - \xi))}{\tanh (\beta \xi) + \tanh (\beta (1 - \xi))} \quad (5)$$
where \( \xi \in [0, 1] \) and \( \beta \) are the threshold and projection parameters for the threshold projection, respectively. On the choice of the values of \( \xi \) and \( \beta \), one can refer to [40][41].

EOT is featured by its high transmission of the photonic energy through periodic subwavelength metallic apertures. The input and output transmission power for one period of the metallic slits can be measured by the integration of the average Poynting vector on the the inlet and outlet sides of the computational domain

\[
P_i = \int_{\Gamma_i} -\frac{1}{2} \text{Re}(E_i \times H_i^*) \cdot n \, d\Gamma = \int_{\Gamma_i} \text{Re} \left( \frac{1}{2j\omega \epsilon_{\infty} \mu_0} H_{zi}^* \nabla H_{zi} \right) \cdot n \, d\Gamma
\]

(6)

\[
P_o = \int_{\Gamma_o} \frac{1}{2} \text{Re}(E \times H^*) \cdot n \, d\Gamma = \int_{\Gamma_o} \text{Re} \left( \frac{-1}{2j\omega \epsilon_{\infty} \mu_0} (H_{zi} + H_{zs})^* \nabla (H_{zi} + H_{zs}) \right) \cdot n \, d\Gamma
\]

(7)

where \( P_i \) and \( P_o \) are the input and output transmission power, respectively; \( E_i \) is the electric fields corresponding to the incident magnetic wave \( H_i = (0, 0, H_{zi}) \); \( E \) is the total electric fields; \( H \) is the total magnetic fields; \( \text{Re} \) operator is used to extract the real part of an expression; * represents the conjugate of the complex variable. The objective of the inverse design procedure can be chosen to maximize the transmissivity defined as the normalized transmission power

\[
T_r = P_o / P_i
\]

(8)

Then the inverse design problem for the bilateral nanostructures of periodic metallic slits is to maximize the transmissivity defined in Eqn. (8) which is constrained by Eqn. (1) and Eqn. (4) with design variable valued in \([0, 1]\). The gradient-based iterative procedure, method of moving asymptotes [35], is applied to update the design variable and maximize the transmissivity. And the gradient information is obtained using the continuous adjoint method [12]

\[
\delta T_r = \int_{\Omega} -\text{Re}(\tilde{\rho}_a^*) \delta \rho \, d\Omega
\]

(9)

where \( \tilde{\rho}_a \) is the adjoint of the filtered design variable \( \tilde{\rho} \). \( \tilde{\rho}_a \) is derived by solving the adjoint equations of the wave equation in Eqn. (1) and density filter in Eqn. (4)

\[
\int_{\Omega} -\epsilon_r^{-1} \nabla \tilde{H}_{zs}^* \cdot \nabla \phi + k_0^2 \mu_r \tilde{H}_{zs}^* \phi \, d\Omega + \int_{\Gamma_o} \left( -j k_0 \sqrt{\epsilon_r^{-1} \mu_r} \tilde{H}_{zs}^* + \frac{1}{P_i} \frac{\partial B}{\partial H_{zs}} \right) \phi \, d\Gamma
\]

\[
+ \int_{\Gamma_o} \frac{1}{P_i} \frac{\partial B}{\partial H_{zs}} \cdot \nabla \phi \, d\Gamma = 0, \forall \phi \in \mathcal{H}^1(\Omega)
\]

(10)

\[
\int_{\Omega_d} r^2 \nabla \tilde{\rho}_a \cdot \nabla \psi + \left[ \tilde{\rho}_a^* - \frac{\partial \epsilon_r^{-1} \partial \tilde{\rho}}{\partial \rho} \nabla (H_{zs} + H_{zi}) \cdot \nabla \tilde{H}_{zs}^* \right] \psi \, d\Omega = 0, \forall \psi \in \mathcal{H}^1(\Omega_d)
\]

(11)

where \( \tilde{H}_{zs} \) and \( B \) represent the adjoint of \( H_{zs} \) and the integral function of Eqn. (7) respectively; \( \mathcal{H}^1(\Omega) \) and \( \mathcal{H}^1(\Omega_d) \) are the first order Hilbert functional spaces defined on \( \Omega \) and \( \Omega_d \).

### 3 Results and discussion

Using the outlined topology optimization based inverse design procedure for enhancing EOT of periodic metallic slits, the bilateral nanostructures are investigated as follows. The noble metal is chosen to be Ag, with high-frequency bulk permittivity \( \epsilon_{\infty} = 6 \), bulk plasmon frequency \( \omega_p = 1.5 \times 10^{16} \text{ rad/s} \), and collision frequency \( \gamma_c = 7.73 \times 10^{13} \text{ rad/s} \) derived by fitting the experimental data in the literatures [43]. The sizes of the computational domain shown in Fig. 1 are set to be the typical values: 1050nm for the periodic length of the metallic slits, 40nm for the slit width, 350nm for the thickness of the fixed Ag layer \( \Omega_m \), and 350nm for the thickness of the design domain \( \Omega_d \) (Fig. 2). The incident wavelength is scanned in the visible light region (350 ~ 770 nm). For different incident wavelengths, the nanostructures sticking to the metallic slits are...
derived as shown in Fig. 3a–f, with corresponding magnetic field distribution shown in Fig. 4a–f. These results demonstrate that the inversely derived nanostructures sticking to the inlet side of the subwavelength slits excite SPPs and guide the SPPs propagating into the metallic slits; the two streams of SPPs in the slits propagate along the two sides of the metallic slits, couple with each other, the Fabry-Pérot resonance of these two streams of SPPs is established sequentially with strengthened transmission [44–48]; at the outlet side, the resonating SPPs is scattered and radiated into free space by the inversely derived nanostuctures; at last, EOT is achieved and enhanced by the inversely designed bilateral nanostructures, with resonance peaks demonstrated in the transmission spectra shown in Fig. 5.

Figure 2: Size presetting of the periodic metallic slits.

Figure 3: Inversely designed bilateral nanostructures for the periodic metallic slits with extraordinary optical transmission corresponding to different incident wavelengths in the visible light region.

The effectivity of the inversely designed bilateral nanostructures on enhancing the EOT performance of periodic metallic slits can be demonstrated furthermore by the transmission spectra in Fig. 5. There are two transmission peaks at the wavelength 526nm and 616nm for the periodic metallic slits without bilateral nanostructures. These transmission peaks are enhanced 3.27 and 4.06 times respectively by the inversely designed bilateral nanostructures with geometrical configurations shown in Fig. 3c and 3d.
In Fig. 5, the transmission peaks are presented at the specified incident wavelengths in the inverse design procedure, and the peak is red shifted along with the increase of the incident wavelength. Therefore, the derived nanostructures result in the resonant EOT performance at the specified incident wavelength, i.e. the nanostructures derived by the inverse design method are resonant for EOT of periodic metallic slits. Sequentially, this inverse design method can be used to control the presentation of the transmission peak at a desired frequency, by specifying the incident wavelength corresponding to the desired frequency in the inverse design procedure.

The transmission spectra in Fig. 5 also demonstrates that the transmission peak is raised along with the red shift of the incident wavelength. This is mainly caused by the large absorption of the photonic energy and short propagation distance of SPP in the short-wavelength region, and relatively low absorption and long propagation distance of SPP in the long-wavelength region. And this can be confirmed by the comparison of transmission, reflection and absorption spectra of the periodic metallic slits with inversely designed bilateral nanostructures (Fig. 6). The absorption spectra in Fig. 6 also demonstrate that the periodic metallic slits with inversely derived bilateral nanostructures have resonant light absorption performance, e.g. 95% of the photonic energy is absorbed by the slits shown in Fig. 3b at the incident wavelength 390nm.

The discussed inverse design method can be extended to enlarge the EOT bandwidth of the periodic metallic slits. And by enlarge the EOT bandwidth, the sensitivity of the transmissivity to the incident wavelengths can be reduced in a specified wavelength range. Then one maximum - minimum inverse design objective is formulated for the bilateral nanostructures of the periodic metallic slits at a central incident wavelength with specified wavelength perturbation range

$$\max_{\rho \in [0,1]} \left\{ \min_{\lambda \in [\lambda_0 - \frac{\theta}{2}, \lambda_0 + \frac{\theta}{2}]} T_r(\lambda) \right\}$$  \hspace{1cm} (12)$$

where $\lambda_0$ is the central incident wavelength; $\theta$ is the support size of the wavelength perturbation range. By respectively setting the central incident wavelength and support size to be 526 and 80nm, the geometrical configuration of the periodic metallic slits is derived as shown in Fig. 7a, where the magnetic field distribution corresponding to...
Figure 5: Transmission spectra of the periodic metallic slits with inversely designed bilateral nanostructures shown in Fig. 3 and the periodic metallic slits without bilateral nanostructures. There are two transmission peaks at the wavelength 526nm and 616nm for the periodic metallic slits without bilateral nanostructures. By the inverse design method, these transmission peaks are enhanced 3.27 and 4.06 times, respectively. The transmission peaks of the periodic metallic slits with inversely designed bilateral nanostructures are presented at the specified incident wavelengths used in the inverse design procedure.

Figure 6: Transmission, reflection and absorption spectra of the periodic metallic slits respectively corresponding to the geometrical configurations shown in Fig. 3a∼f, where large absorption is presented in the short-wavelength region, and relatively low absorption is presented as the red sift of the wavelength.
the minimum transmissivity at the wavelength 504nm is included; and the transmission spectra of the derived periodic metallic slits is shown in Fig. 7. When the central incident wavelength is changed to be 616nm, the geometrical configuration shown in Fig. 8 is derived for the TM wave with incident wavelength in the range from 576 to 656nm, where the magnetic field distribution corresponding to the minimum transmissivity at the wavelength 576nm is included; and the corresponding transmission spectra is shown in Fig. 8. The transmission spectra in Fig. 7 and 8, demonstrate that EOT is controlled to be less sensitive to the incident wavelength with the cost of decreasing transmissivity and it is feasible to enlarge the EOT bandwidth of subwavelength structures using the discussed inverse design method.

Figure 7: (a) Periodic metallic slits with inversely designed bilateral nanostructures for the TM wave with incident wavelength in the range from 486 to 566nm, and the corresponding magnetic field distribution in the derived metallic slit configuration corresponding to the minimum transmissivity at the wavelength 504nm in the prescribed wavelength range; (b) transmission spectra of the derived metallic slit configuration, where the spectra of the periodic metallic slits with bilateral nanostructures inversely designed at the central wavelength of the wavelength range and that of the periodic metallic slits without bilateral nanostructures are included.

4 Conclusion

This paper has presented inversely determining the resonant configuration of the bilateral nanostructures for periodic metallic slits with extraordinary optical transmission performance. The topology optimization approach is utilized to implement the inverse design procedure. Several geometrical configurations of the bilateral nanostructures are derived for periodic metallic slits. The resonant performance of the derived nanostructures are demonstrated by the transmission spectra, where the transmission peak is presented at the specified wavelength in the inverse design procedure. This provides an approach to control the red or blue shift of the transmission peak or localize the resonant performance at a desired frequency, by specifying the desired incident wavelength in the inverse design procedure. The inverse design method is extended to make the periodic metallic slits to be less sensitive to the incident wavelength. This research can be further extended to inversely find the resonant subwavelength structures for extraordinary optical absorption and other surface palson polariton based photonic devices. The inverse design of three dimensional apertures for extraordinary optical transmission will be investigated in our future researches.

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Figure 8: (a) Periodic metallic slits with inversely designed bilateral nanostructures for the TM wave with incident wavelength in the range from 576 to 656nm, and the corresponding magnetic field distribution in the derived metallic slit configuration corresponding to the minimum transmissivity at the wavelength 576nm in the prescribed wavelength range; (b) transmission spectra of the derived metallic slit configuration, where the spectra of the periodic metallic slits with bilateral nanostructures inversely designed at the central wavelength of the wavelength range and that of the periodic metallic slits without bilateral nanostructures are included.

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