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RESEARCH ARTICLE

Functional control of anomalous reflection via engineered metagratings without polarization limitations

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Supporting Information

1. Specific derivation details of the formulas in the manuscript, including Note 1 and Note 2

Note 1 Diffraction theory of inversely-designed metegratings for TM waves

1.1 The diffraction theory for TM waves

A transverse Magnetic (TM) plane wave illuminates on the grating (see Fig. 1(a)), where the metal is considered as perfect electric conductor (PEC) and there are multiple reflection diffraction orders governed by the grating equation. In the incident region ($z < 0$), the magnetic and electric field components can be written as

$$H_y = \sum_n (\delta_{n,0} e^{ik_z^n z} + R_n e^{-ik_z^n z})\, e^{ik_x^n x}, \tag{S1-1}$$

$$E_x = \frac{1}{k_0 c\varepsilon} \sum_n k_z^n (\delta_{n,0} e^{ik_z^n z} - R_n e^{-ik_z^n z})\, e^{ik_x^n x}, \tag{S1-2}$$

where, $\delta_{n,0}$ is Kronecker delta, k_0 is the wave vector in free space,c is the speed of light in vacuum, ε is the material dielectric constant, R_n is the complex amplitude of n^{th} diffraction order, $k_x^n = k_0 + 2\pi n/p$ is the wave vector in the x-direction, $k_z^n = \sqrt{(k_0^2) - (k_x^n)^2}$ is the wave vector in the z-direction.

Considering a subwavelength groove with width w and depth L, the electromagnetic field in the groove can be written as

$$H_{y,m} = A_m \cos(m\pi x/w) \cos(\beta_m (z - L)), \tag{S1-3}$$

$$E_{x,m} = \frac{i}{k_0 c\varepsilon} \beta_m A_m \cos(m\pi x/w) \sin(\beta_m (z - L)), \tag{S1-4}$$

where, A_m is the complex amplitude, $k_x^m = m\pi/w$ is the transverse wave vector, and $\beta_m = \sqrt{k_0^2 - (k_x^m)^2}$ is the propagation constant for m^{th} waveguide mode. Considering the boundary condition of magnetic field at $z = 0$, Eq. (S1-1) and Eq. (S1-3) can be written as

$$H_y = \sum_n (\delta_{n,0} + R_n)\, e^{ik_x^n x}, \tag{S1-5}$$

$$H_{y,m} = A_m \cos\left(\frac{m\pi x}{w}\right) \cos(\beta_m L). \tag{S1-6}$$

Considering the orthogonality of different diffraction orders, we multiply Eq. (S1-5) and Eq. (S1-6) by $\cos(m\pi x/w)$ and then integrate over $0 < x < w$ respectively. It yields

$$\sum_n (\delta_{n,0} + R_n) \int_0^w e^{ik_x^n x} \cos(m\pi x/w)\, \mathrm{d}x = A_m \cos(\beta_m L) \int_0^w \cos^2(m\pi x/w)\, \mathrm{d}x. \tag{S1-7}$$

The integral term in Eq. (S1-7) can be written as

$$\int_0^w \cos^2(m\pi x/w)\mathrm{d}x = \int_0^w \frac{1}{2}[1+\cos\left(\frac{2m\pi x}{w}\right)]dx = \frac{w}{2}(\delta_{m,0}+1), \tag{S1-8}$$

$$\int_0^w e^{ik_x^n x}\cos(m\pi x/w)dx = \frac{ik_x^n[\exp(ik_x^n w)\cos(m\pi)-1]}{(m\pi/w)^2-(k_x^n)^2} = M_{m,n}. \tag{S1-9}$$

Eq. (S1-7) can be simplified as

$$\sum_n(\delta_{n,0}+R_n)\,M_{m,n} = \frac{w}{2}(\delta_{m,0}+1)A_m\cos(\beta_m L). \tag{S1-10}$$

The boundary condition for electric field is considered at $z=0$, Eq. (S1-2) and Eq. (S1-4) can be written as

$$E_x = \frac{1}{k_0 c\varepsilon}\sum_n k_z^n(\delta_{n,0}-R_n)\,e^{ik_x^n x}, \tag{S1-11}$$

$$E_{x,m} = -\frac{i}{k_0 c\varepsilon}\beta_m A_m\cos\left(\frac{m\pi x}{w}\right)\sin(\beta_m L). \tag{S1-12}$$

Considering the orthogonality of different diffraction orders, we multiply Eq. (S1-11) and Eq. (S1-12) by $e^{-ik_x^n x}$ and then integrate over $0<x<p$ respectively. It yields

$$\int_0^p \frac{1}{k_0 c\varepsilon}\sum_n k_z^n(\delta_{n,0}-R_n)\,e^{ik_x^n x}e^{-ik_x^n x}\mathrm{d}x = \sum_m \int_0^w \frac{i}{k_0 c\varepsilon}\beta_m A_m\cos\left(\frac{m\pi x}{w}\right)\sin(\beta_m L)\,e^{-ik_x^n x}\mathrm{d}x. \tag{S1-13}$$

The integral term in Eq. (S1-13) can be written as

$$N_{m,n} = \int_0^w \cos\left(\frac{m\pi x}{w}\right)e^{-ik_x^n x}dx = M_{m,n}^*. \tag{S1-14}$$

Eq. (S1-13) can be simplified as

$$ipk_z^n(\delta_{n,0}-R_n) = \sum_m \beta_m A_\mathrm{m}\sin(\beta_m L)\,N_{m,n}. \tag{S1-15}$$

Eqs. (S1-10) and (S1-15) constitute a complete set of linear algebraic problems with the parameters k_0, w, L, and p provided and set truncation of n and m. The reflection coefficient R_n and the amplitude in the groove A_m of the MG can be derived.

1.2 The inverse-design equations of $R_0^{\mathrm{TM}}=0$ and $R_{-1}^{\mathrm{TM}}=0$ for considering β_0 and β_1

Considering the designed MG with the evanescent first-order guided mode, $m=1$. We notice that the definition of the parameter in Eq. (S1-10) is different from that in Eq. (S1-15). Therefore, we rewrite 'm' in Eq. (S1-10) as 'm'', while keeping 'm' unchanged in Eq. (S1-15).

Then Eq. (S1-10) and Eq. (S1-15) can be written as

$$\sum_n(\delta_{n,0}+R_n)\,M_{m',n} = \frac{w}{2}(\delta_{m',0}+1)A_{m'}\cos(\beta_{m'}L), \tag{S1-16}$$

$$ipk_z^n(\delta_{n,0}-R_n) = \sum_m \beta_m A_\mathrm{m}\sin(\beta_m L)\,N_{m,n}. \tag{S1-17}$$

Considering the retroreflection conditions $R_0=0$ in Eq. (S1-17), we get

$$ipk_z^0 = \beta_0 A_0\sin(\beta_0 L)\,N_{0,0} + \beta_1 A_1\sin(\beta_1 L)\,N_{1,0}. \tag{S1-18}$$

We multiply Eq. (S1-17) by $M_{m',n}/(ipk_z^n)$ and then summate from n. Eq. (S1-16) plus the result of the summation, after simplification, we get

$$2M_{m',0} = \frac{w}{2}\left(\delta_{m',0}+1\right)A_{m'}\cos(\beta_{m'}L) + \sum_n\left(\frac{M_{m',n}}{ipk_z^0}\sum_m \beta_m\sin(\beta_m L)\,N_{m,n}\right). \tag{S1-19}$$

Expanding Eq. (S1-19), we can obtain

$$2M_{0,0} = wA_0\cos(\beta_0 L) + A_0\beta_0\sin(\beta_0 L)\sum_n\frac{M_{0,n}N_{0,n}}{ipk_z^n} + A_1\beta_1\sin(\beta_1 L)\sum_n\frac{M_{0,n}N_{1,n}}{ip\ _z^n}, \tag{S1-20}$$

$$2M_{1,0} = \frac{w}{2}A_1\cos(\beta_1 L) + A_0\beta_0\sin(\beta_0 L)\sum_n\frac{M_{1,n}N_{0,n}}{ipk_z^n} + A_1\beta_1\sin(\beta_1 L)\sum_n\frac{M_{1,n}N_{1,n}}{ipk_z^n}. \tag{S1-21}$$

The complex amplitude A_0 and A_1 can be solved by Eqs. (S1-20) and (S1-21). Taking the solution into Eq. (S1-18) and using retroreflection conditions $k_x^0 = -k_x^{-1}$, $k_z^0 = k_z^{-1}$ it yields, the new inverse-design condition of perfect retroreflection is written as

$$\frac{w^2}{2}\cot(\beta_0 L)\cot(\beta_1 L) + C_1 w\cot(\beta_0 L)\,\beta_1 + C_2 w\cot(\beta_1 L)\,\beta_0 = C_3\beta_0\beta_1, \tag{S1-22}$$

where the coefficients C_1, C_2 and C_3 are written as

$$\begin{cases} C_1 = D'_{1,1} \\ C_2 = \frac{1}{2}D'_{0,0} \\ C_3 = D_{1,1}\left(D_{0,0} - D'_{0,0}\right) - D'_{1,1}D_{0,0} + D_{1,0}\left(D_{0,1} - 2D'_{0,1}\right) - 2D'_{1,0}D_{0,1} \end{cases}, \tag{S1-23}$$

where $D_{m,m'} = \sum_n \frac{M_{m,n}N_{m',n}}{ipk_z^n}$ and $D'_{m,m'} = \sum_{n\neq 0,-1} \frac{M_{m,n}N_{m',n}}{ipk_z^n}$.

Considering specular-reflection conditions $R_{-1} = 0$ in Eq. (S1-17), it yields

$$\beta_0 A_0 \sin(\beta_0 L)\, N_{0,-1} + \beta_1 A_1 \sin(\beta_1 L)\, N_{1,-1} = 0. \tag{S1-24}$$

The complex amplitude A_0 and A_1 can be solved by Eqs. (S1-20) and (S1-21). Taking the solution into Eq. (S1-23) and using retroreflection conditions $k_x^0 = -k_x^{-1}$, $k_z^0 = k_z^{-1}$ it yields, the new inverse-design condition of perfect specular-reflection is written as

$$\beta_0 N_{0,-1}\left(2M_{0,0}\left[\frac{w}{2}\cot(\beta_1 L) + \beta_1\sum_n \frac{M_{1,n}N_{1,n}}{ipk_z^n}\right] - 2M_{1,0}\beta_1\sum_n \frac{M_{0,n}N_{1,n}}{ipk_z^n}\right)$$

$$+\beta_1 N_{1,-1}\left(2M_{1,0}\left[w\cot(\beta_0 L) + \beta_0\sum_n \frac{M_{0,n}N_{0,n}}{ipk_z^n}\right] - 2M_{0,0}\beta_0\sum_n \frac{M_{1,n}N_{0,n}}{ipk_z^n}\right) = 0^{\dagger}. \tag{S1-25}$$

1.3 The inverse-design equations of $R_0^{\mathrm{TM}} = 0$ and $R_{-1}^{\mathrm{TM}} = 0$ for considering β_0

Considering the designed MG with only the fundamental mode of propagation, $m = 0$. Then Eq. (S1-10) and Eq. (S1-15) can be written as

$$\sum_n\left(\delta_{n,0} + R_n\right)M_{0,n} = wA_0\cos(\beta_0 L), \tag{S1-26}$$

$$ipk_z^n\left(\delta_{n,0} - R_n\right) = \beta_0 A_0\sin(\beta_0 L)\, N_{0,n}. \tag{S1-27}$$

Considering retroreflection conditions $R_0 = 0$ in Eq. (S1-27), it yields

$$ipk_z^0 = A_0\sin(\beta_0 L)N_{0,0}\beta_0. \tag{S1-28}$$

Operating on the above equations with Eq. (S1-24) $+\sum_n$[Eq. (S1-25) $\times\, M_{0,n}/(ipk_z^n)$], after simplification, we get

$$2M_{0,0} = wA_0\cos(\beta_0 L) + \frac{\beta_0 A_0\sin(\beta_0 L)}{ip}\sum_n \frac{M_{0,n}N_{0,n}}{k_z^n}. \tag{S1-29}$$

Replace the term A_0 in Eq. (S1-29) by Eq. (S1-28),

$$2M_{0,0} = \frac{ipk_z^0 w}{N_{0,0}\beta_0}\cot(\beta_0 L) + \frac{k_z^0}{N_{0,0}}\sum_n \frac{M_{0,n}N_{0,n}}{k_z^n}. \tag{S1-30}$$

It can be simplified as

$$\cot(\beta_0 L) = \frac{\beta_0}{ipw}\left[\frac{2M_{0,0}N_{0,0}}{k_z^0} - \sum_n \frac{M_{0,n}N_{0,n}}{k_z^n}\right]. \tag{S1-31}$$

The MN term in Eq. (S1-31) can be written as

$$M_{0,n}N_{0,n} = w^2\mathrm{sinc}^2\left(\frac{k_x^n w}{2}\right). \tag{S1-32}$$

Due to the retroreflection conditions $k_x^0 = -k_x^{-1}$, $k_z^0 = k_z^{-1}$, it yields

$$M_{0,0}N_{0,0} = M_{0,-1}N_{0,-1}. \tag{S1-33}$$

The reversal design equation of retroreflection for TM waves with fundamental mode can be obtained by taking the condition Eqs. (S1-32) and (S1-33) into Eq. (S1-31),

$$\cot(\beta_0 L) = \frac{iw\ \ _0}{p}\sum_{n\neq 0,-1}\frac{\mathrm{sinc}^2(k_x^n w/2)}{k_z^n}\ . \tag{S1-34}$$

Considering specular-reflection conditions $R_{-1} = 0$ in Eq. (S1-28), it yields

$$A_0\sin(\beta_0 L)N_{0,0}\beta_0 = 0\ . \tag{S1-35}$$

The new inverse-design condition of perfect specular-reflection is written as

$$L = \frac{N\pi}{\beta_0}, (N = 0,1,2\ldots)\ . \tag{S1-36}$$

We use a finite-element numerical simulation software (COMSOL) to further compare the retroreflection performance designed using Eq. (S1-34) (Eq. (3) in the main text) and Eq. (S1-22) (Eq. (2) in the main text). The MG period is for the retroreflection. By employing the theorical design parameters obtained from these two inverse-design methods (see Figs. S1(a) and (b)), we show the corresponding numerical results of retroreflection efficiency in Figs. S1(c) and (d). The results show that Eq. (S1-34) (Eq. (3) in the main text) can be also used to design perfect retroreflection of TM waves except for a larger incident angle and a wider groove width.

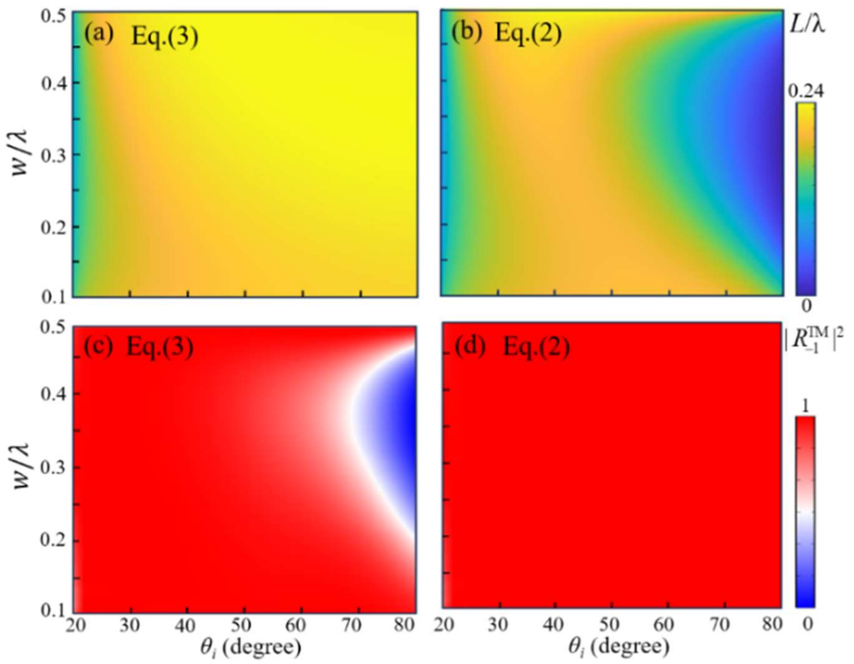

Fig. S1 (a, b) The designed groove depth for perfect retroreflection using Eq. (3) and Eq. (2) for TM polarized waves, respectively. **(c, d)** Analytically calculated retroreflection efficiency $|R_{-1}^{\mathrm{TM}}|^2$ based on the analytical solution in (a) and (b).

Note 2 Diffraction theory of inversely-designed metegratings for TE waves

2.1 The diffraction theory for TE waves

A transverse electric (TE) plane wave illuminates on the grating (see Fig. 1(a)), where the metal is considered as perfect electric conductor (PEC) and there are multiple reflection and transmission diffraction orders governed by the grating equation. The total derivation process is similar as above. For brevity, the repetitive steps will be omitted here.

In the incident region, the magnetic and electric field components can be written as

$$E_y^1 = \sum_n (\delta_{n,0} e^{ik_z^n z} + R_n e^{-ik_z^n z}) e^{ik_x^n x}, \tag{S2-1}$$

$$H_x^1 = -\frac{1}{k_0 Z_0} \sum_n k_z^n (\delta_{n,0} e^{ik_z^n z} - R_n e^{-ik_z^n z})\, e^{ik_x^n x}, \tag{S2-2}$$

where, Z_0 is the impedance. Owing to the effect of PEC, the electromagnetic field in the groove can be written as

$$E_y = A_m \sin(m\pi x/w) \sin(\beta_m(z-L)), \tag{S2-3}$$

$$H_x = \frac{i}{k_0 Z_0} \sum_m \beta_m \mathrm{A_m} \sin(m\pi x/w) \cos(\beta_m(z-L)), \tag{S2-4}$$

where, A_m is the complex amplitude of m^{th} waveguide mode.

The boundary condition for electric field is considered at $z = 0$ yields, Eq. (S2-1) and Eq. (S2-3) can be written as

$$E_y^1 = \sum_n (\delta_{n,0} + R_n)\, e^{ik_x^n x}, \tag{S2-5}$$

$$E_y = -A_m \sin\left(\frac{m\pi x}{w}\right) \sin(\beta_m L). \tag{S2-6}$$

Considering the orthogonality of different diffraction orders, we multiply Eq. (S2-5) and Eq. (S2-6) by $e^{-ik_x^n x}$and then integrate over $0 < x < p$ respectively. It yields

$$p(\delta_{n,0} + R_n) = -\int_0^w \sum_m A_m \sin\left(\frac{m\pi x}{w}\right) \sin(\beta_m L)\, e^{-ik_x^n x} dx. \tag{S2-7}$$

The integral term in Eq. (S2-7) can be written as

$$C_{n,m}^- = \frac{1}{p}\int_0^w \sin(m\pi x/w)\, e^{-ik_x^n x} dx = \frac{1}{p}\frac{m\pi}{w}\frac{1-e^{-ik_x^n w}\cos(m\pi)}{(\frac{m\pi}{w})^2-(k_x^n)^2}. \tag{S2-8}$$

Eq. (S2-7) can be simplified as

$$\delta_{n,0} + R_n = -\sum_m A_m \sin(\beta_m L)\, C_{n,m}^-. \tag{S2-9}$$

The boundary condition of magnetic field at $z = 0$, Eq. (S2-2) and Eq. (S2-4) can be written as

$$H_x^1 = -\frac{1}{k_0 Z_0} \sum_n k_z^n (\delta_{n,0} - R_n)\, e^{ik_x^n x}, \tag{S2-10}$$

$$H_x = \frac{i}{k_0 Z_0} \sum_m \beta_m \mathrm{A_m} \sin(m\pi x/w) \cos(\beta_m L). \tag{S2-11}$$

Considering the orthogonality of different diffraction orders, we multiply Eq. (S2-10) and Eq. (S2-11) by $\sin(m\pi x/w)$ and then integrate over $0 < x < w$ respectively. It yields

$$-\int_0^w \sum_n (\delta_{n,0} - R_n)\, k_z^n e^{ik_x^n x} \sin(m\pi x/w) dx = i\frac{w}{2} A_m \beta_m \cos(\beta_m \mathrm{L}). \tag{S2-12}$$

The integral term in Eq. (S2-12) can be written as

$$ik_z^n \int_0^w e^{ik_x^n x} \sin(m\pi x/w) dx = ik_z^n \frac{m\pi}{w}\frac{1-e^{ik_x^n w}\cos(m\pi)}{(\frac{m\pi}{w})^2-(k_x^n)^2} = C_{n,m}^+. \tag{S2-13}$$

Eq. (S2-12) can be simplified as

$$\sum_n (\delta_{n,0} - R_n)\, C_{n,m}^+ = \frac{w}{2} A_m \beta_m \cos(\beta_m \mathrm{L}). \tag{S2-14}$$

Eqs. (S2-9) and (S2-14) constitute a complete set of linear algebraic problems. With the parameters k_0, w, L and p provided and set the truncation of n and m, we can derive the reflection coefficient R_n and the amplitude in the groove A_m of the MG.

2.2 The inverse-design scheme of $R_0^{\mathrm{TE}} = 0$ and $R_{-1}^{\mathrm{TE}} = 0$ for considering β_1

Considering the designed MG with the fundamental mode of propagation TE, $m = 1$. Then Eq. (S2-9) and Eq. (S2-14) can be written as

$$\delta_{n,0} + R_n = -A_1 \sin(\beta_1 L) C_{n,1}^-, \tag{S2-15}$$

$$\sum_n \left(\delta_{n,0} - R_n\right) C_{n,1}^{+} = \frac{w}{2} A_1 \beta_1 \cos(\beta_1 \mathrm{L}). \tag{S2-16}$$

Operating on the above equations with $\sum_n$ Eq. (S2 − 15) plus Eq. (S2-16), we get

$$2C_{0,1}^{+} = \frac{w}{2} A_1 \beta_1 \cos(\beta_1 \mathrm{L}) - A_1 \sin(\beta_1 L) \sum_n C_{n,1}^{-} C_{n,1}^{+}. \tag{S2-17}$$

Considering retroreflection conditions $R_0 = 0$ in Eq. (S2-15), it yields

$$1 = -A_1 \sin(\beta_1 L)\, C_{0,1}^{-}. \tag{S2-18}$$

Replace the term A_1 in Eq. (S2-17) by Eq. (S5-18),

$$2C_{0,1}^{+} C_{0,1}^{-} = -\frac{w}{2} \beta_1 \cot(\beta_1 \mathrm{L}) + \sum_n C_{n,1}^{-} C_{n,1}^{+}. \tag{S2-19}$$

It can be simplified as

$$\frac{w}{2} \beta_1 \cot(\beta_1 \mathrm{L}) = \sum_n C_{n,1}^{-} C_{n,1}^{+} - 2C_{0,1}^{+} C_{0,1}^{-}. \tag{S2-20}$$

The $C_{n,1}^{-} C_{n,1}^{+}$ term in Eq. (S2-20) can be written as

$$C_{n,1}^{-} C_{n,1}^{+} = \frac{ik_z^n}{p} \left(\frac{\pi}{w}\right)^2 \frac{2+2\mathrm{co}\ \ (k_x^n w)}{\left(\left(\frac{\pi}{w}\right)^2 - (k_x^n)^2\right)^2}. \tag{S2-21}$$

Considering retroreflection conditions $k_x^0 = -k_x^{-1}$, $k_z^0 = k_z^{-1}$, it yields

$$C_{0,1}^{-} C_{0,1}^{+} = C_{-1,1}^{-} C_{-,1}^{+}. \tag{S2-22}$$

The reversal design equation of retroreflection for TE waves with fundamental mode can be obtained by taking the condition Eqs. (S2-21) and (S2-22) into Eq. (S2-20),

$$\frac{w}{2} \beta_1 \cot(\beta_1 \mathrm{L}) = \frac{2i}{p} \left(\frac{\pi}{w}\right)^2 \sum_{n \neq 0,-1} k_z^n \frac{1+\cos\,(k_x^n w)}{\left(\left(\frac{\pi}{w}\right)^2 - (k_x^n)^2\right)^2}\ . \tag{S2-23}$$

Considering specular-reflection conditions $R_{-1} = 0$ in Eq. (S2-15), it yields

$$-A_1 \sin(\beta_1 L) C_{-1,1}^{-} = 0\ . \tag{S2-24}$$

The new inverse-design condition of perfect specular-reflection is written as

$$L = \frac{N\pi}{\beta_1}, (N = 0,1,2 \ldots)\ . \tag{S2-25}$$

2.3 The inverse-design scheme of $R_0^{\mathrm{TE}} = 0$ for considering $\boldsymbol{\beta_1}$ and $\boldsymbol{\beta_2}$

Considering the designed MG with the evanescent first-order guided mode, $m = 2$. We notice that the definition of the parameter in Eq. (S2-9) is different from that in Eq. (S2-14). Therefore, we rewrite '*m*' in Eq. (S2-9) as '*m*'', while keeping '*m*' unchanged in Eq. (S2-14).

Then Eq. (S2-17) can be written as

$$2C_{0,m'}^{+} = \frac{w}{2} A_{m'} \beta_{m'} \cos(\beta_{m'} \mathrm{L}) - \sum_m A_m \sin(\beta_m L)\, C_{n,m}^{-} C_{n,m}^{+}. \tag{S2-26 }$$

Expanding Eq. (S2-26), we can obtain

$$2C_{0,1}^{+} = \frac{w}{2} A_1 \beta_1 \cos(\beta_1 \mathrm{L}) - A_1 \sin(\beta_1 L)\, D_{1,1} - A_2 \sin(\beta_2 L)\, D_{2,1}, \tag{S2-27 }$$

$$2C_{0,2}^{+} = \frac{w}{2} A_2 \beta_2 \cos(\beta_2 \mathrm{L}) - A_1 \sin(\beta_1 L)\, D_{1,2} - A_2 \sin(\beta_2 L)\, D_{2,2}. \tag{S2-28}$$

Due to the retroreflection conditions $R_0 = 0$ in Eq. (S2-14), we can obtain

$$\delta_{n,0} + R_n = -A_1 \sin(\beta_1 L)\, C_{n,1}^{-} - A_2 \sin(\beta_2 L)\, C_{n,2}^{-}. \tag{S2-29}$$

The complex amplitude A_1 and A_2 can be solved by Eqs. (S2-27) and (S2-28). Taking the solution into Eq. (S2-29) and using retroreflection conditions $k_x^0 = -k_x^{-1}$, $k_z^0 = k_z^{-1}$, the new inverse-design condition of perfect retroreflection is written as

$$\frac{w^2}{4}\beta_1\beta_2 \cot(\beta_1 \mathrm{L})\cot(\beta_2 \mathrm{L}) - F_1\frac{w}{2}\beta_1\cot(\beta_1 \mathrm{L}) - F_2\frac{w}{2}\beta_2 \cot(\beta_2 \mathrm{L}) = F_3, \tag{S2-30}$$

where the coefficients F_1, F_2 and F_3 are written as

$$\begin{cases} F_1 = D'_{2,2} \\ F_2 = D'_{1,1} \\ F_3 = D_{1,1}D_{2,2} + D_{1,2}^2 - D'_{1,1}D_{2,2} - D_{1,1}D'_{2,2} - 2D'_{1,2}D_{1,2} \end{cases}, \tag{S2-31}$$

with $D_{m,m'} = \sum_n C_{n,m}^- C_{n,m'}^+$ and $D'_{m,m'} = \sum_{n\neq 0,-1} C_{n,m}^- C_{n,m'}^+$.

We use a finite-element numerical simulation software (COMSOL) to further compare the retroreflection performance designed using Eq. (S1-30) (Eq. (4) in the main text) and Eq. (S1-23) (Eq. (5) in the main text). The MG period is for the retroreflection. By employing the theoretical design parameters obtained from these two inverse-design methods (see Figs. S2(a) and (b)), we show the corresponding numerical results of retroreflection efficiency in Figs. S2(c) and (d). The results show that the MG designed based on Eq. (3) or Eq. (4) both can achieve perfect retroreflection for TE incident wave.

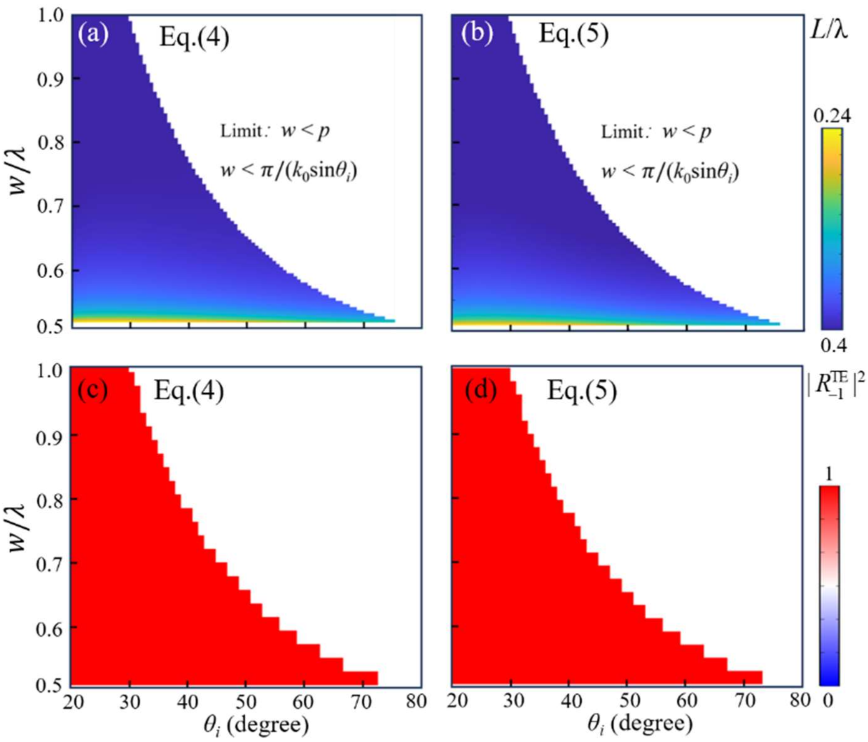

Fig. S2 (a, b) The designed groove depth for perfect retroreflection using Eq. (4) and Eq. (5) for TE polarized waves, respectively. **(c, d)** Analytically calculated retroreflection efficiency $|R_{-1}^{\mathrm{TE}}|^2$ based on the analytical solution in (a) and (b).

2. Supplementary figures to support the contents of Fig. 3, Fig. 4 and Fig. 5 of the main text

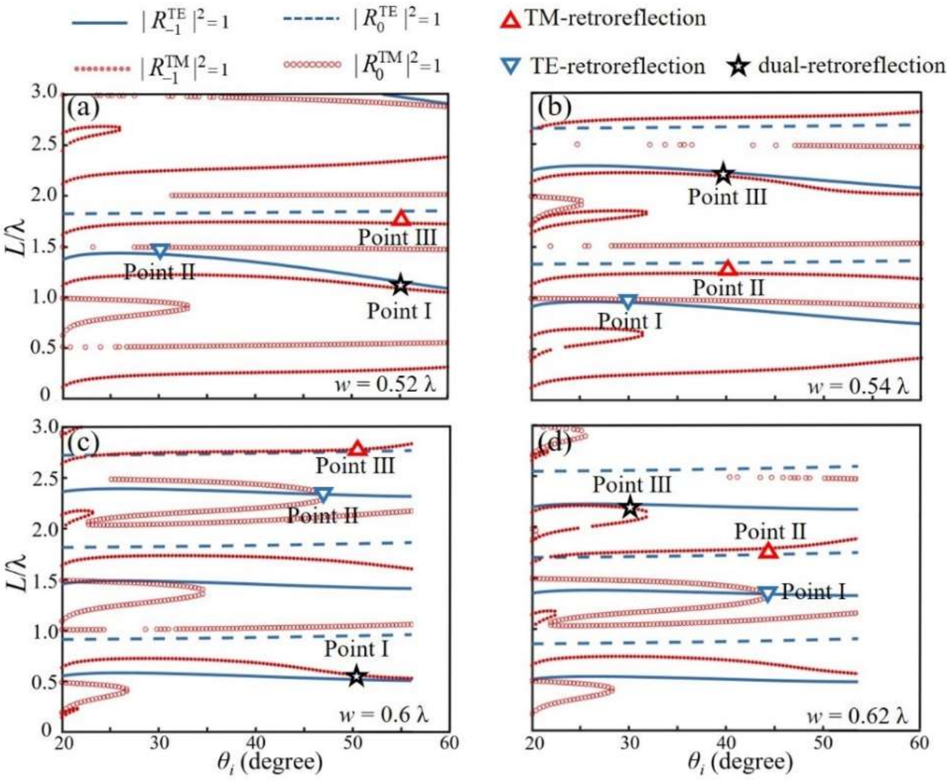

Fig. S3 The analytical solutions for perfect retroreflection (blue curve for TE, red scatter dots for TM) and perfect specular reflection (blue dashed for TE, red hollow dots for TM), in which the working frequency is 2 GHz and **(a)** $w = 0.52\lambda$; **(b)** $w = 0.54\lambda$; **(c)** $w = 0.6\lambda$; **(d)** $w = 0.62\lambda$.

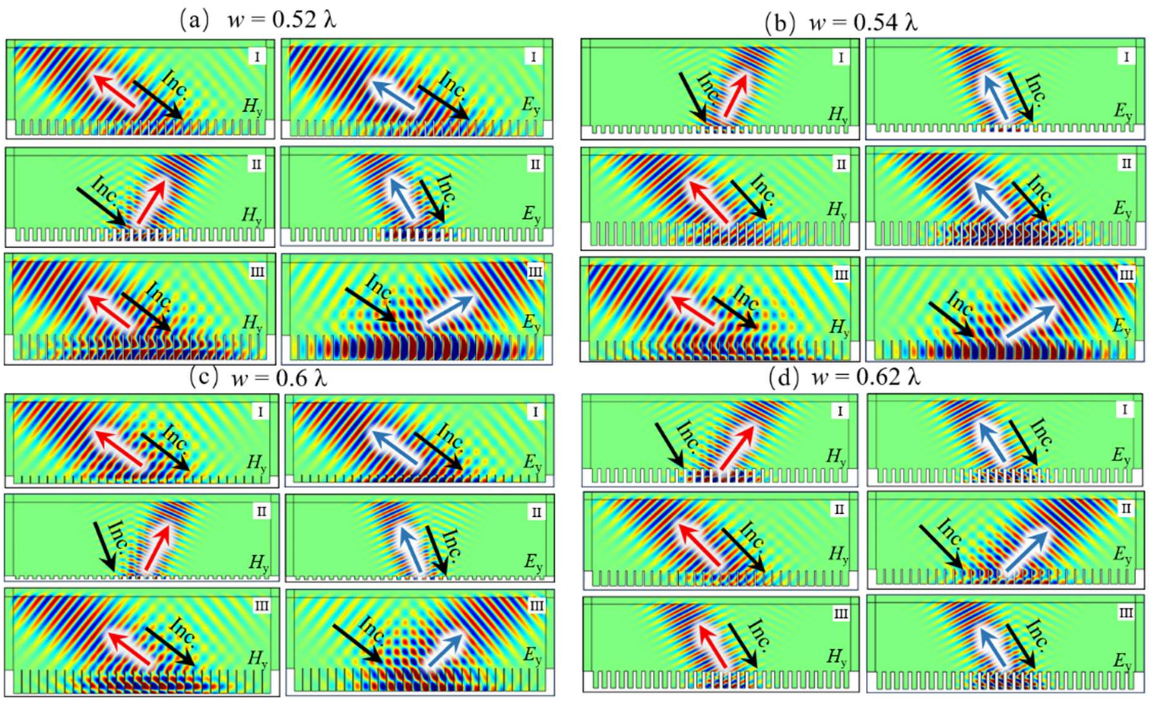

Fig. S4 Simulated scattered field patterns (H_y and E_y) for a Gaussian beam incident on the designed MGs with different groove depth, respectively, in which **(a)** $w = 0.52\lambda$, **(b)** $w = 0.54\lambda$, **(c)** $w = 0.6\lambda$, **(d)** $w = 0.62\lambda$.

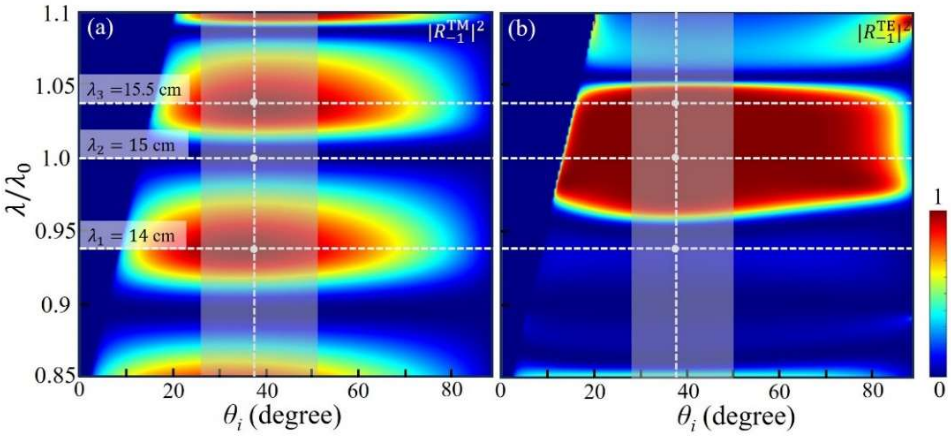

Fig. S5 (a, b) Numerically calculated reflection efficiency of the $n = -1$ order versus the incident angle and the incident wavelength for TM and TE polarized waves. The geometry parameters of the MG are $p = 12.2$ cm, $L = 23.5$ cm, $w = 8.4$ cm.