Supplementary Information

Combined Metagratings for Efficient Broad-Angle Scattering Metasurface

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1. Derivation of the design equations

We use the metagrating theory [1] for a periodic array of horizontally oriented magnetic dipoles. The structure is illuminated with a TM-polarized plane wave propagating in the yz plane:

$$\boldsymbol{E_{inc}} = \boldsymbol{E_0}(\boldsymbol{y}\cos(\boldsymbol{\theta_{inc}}) + \boldsymbol{z}\sin(\boldsymbol{\theta_{inc}}))\, e^{-ik_0(\sin(\theta_{inc})y - \cos(\theta_{inc})z)} \tag{1}$$

with E_0 the amplitude, k_0 the free-space wave number and θ_{inc} the angle of incidence. The magnetic dipoles, induced by the incoming wave have each a magnetic current:

$$\boldsymbol{I_m^x} = -i\omega\alpha_m \boldsymbol{H_{ext}^x} \tag{2}$$

with H_{ext}^x the impinging magnetic field and α_m the effective magnetic particle polarizability. The dipoles are ordered in a periodic array (m×n) with periodicity d_x and d_y in x and y directions, respectively, and are located at a distance h above a ground plane. The magnetic surface current density J_m is the sum of the currents generated by the discrete magnetic dipole moments:

$$\boldsymbol{J_m}(x,y,z) = x I_m^x \delta(z-h) \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \delta(x - md_x)\delta(y - nd_y)\, e^{-ik_0 \sin(\theta_{inc}) n d_y} \,. \tag{3}$$

The Floquet modes into which the array redirects light are the diffraction orders of the given grating condition. To avoid scattering into higher order modes, we first consider the case of 1D periodicity in the y direction and grating geometries with only three Floquet modes n=0, ±1 (first-order diffraction above 30°). The radiated field for Floquet mode n is given by:

$$\boldsymbol{E_n} = \left(y - z\frac{k_0 \sin(\theta_n)}{k_0 \cos(\theta_n)}\right) Q_n \exp(-ik_0 \sin(\theta_n) y - ik_0 \cos(\theta_n) z), \tag{4}$$

with

$$\boldsymbol{Q_n} = \frac{1}{S} \boldsymbol{I_m^x} \cos(\boldsymbol{k_0} \cos(\boldsymbol{\theta_n}) \boldsymbol{h}). \tag{5}$$

S is the area of the unit cells ($S = d_y$ for 1D surface). As energy is conserved and no Ohmic dissipation is considered, the extinction power P_{ext} equals the power re-radiated in all Floquet modes:

$$\boldsymbol{P_{ext}} = \frac{1}{2S} \boldsymbol{Re}\{\boldsymbol{J_m} \cdot \boldsymbol{H_a}\} = \boldsymbol{P_{rad}} = \frac{1}{2\eta_0} \sum_{n=-\infty}^{n=\infty} \frac{1}{\cos \boldsymbol{\theta_n}} |\boldsymbol{Q_n}| \, . \tag{6}$$

Employing equation (2) and (5), (6) can be rewritten as:

$$\boldsymbol{Im}\left\{\frac{1}{\alpha_m}\right\} = \frac{\omega}{\eta_0\, d} \sum_{n=-\infty}^{n=+\infty} \frac{1}{\cos \boldsymbol{\theta_n}} \cos^2(\boldsymbol{k_0 h} \cos(\boldsymbol{\theta_n})). \tag{7}$$

In the radiated fields, the field of the n=0 Floquet mode is:

$$\boldsymbol{E_0} = \left(\boldsymbol{y} - \boldsymbol{z} \frac{\boldsymbol{k_0} \sin(\boldsymbol{\theta_n})}{\boldsymbol{k_0} \cos(\boldsymbol{\theta_n})}\right) \boldsymbol{Q_0} \exp(-\boldsymbol{i k_0} \sin(\boldsymbol{\theta_n}) \boldsymbol{y} - \boldsymbol{i k_0} \cos(\boldsymbol{\theta_n}) \boldsymbol{z}) \tag{8}$$

with $Q_0 = \frac{1}{d} I_m^x \cos(k_0 h)$. To cancel the specular reflection of the incident field from the ground plane with the n=0 Floquet mode the condition $Q_0 = E_0$ has to be fulfilled. Combining this condition with the form of the magnetic current from (2) gives the condition:

$$\frac{\boldsymbol{1}}{\boldsymbol{\alpha_m}} = \frac{\boldsymbol{2 i \omega}}{\boldsymbol{\eta_0\, d}} \cos^2(\boldsymbol{k_0 h}) \tag{9}$$

Now, we assume that only the 0,-1 and +1 grating orders can carry energy. Comparing equation (7) and (9) then leads to the design equation for the cancellation of the specular reflection:

$$\cos^2(\boldsymbol{k_0 h}) = \frac{\boldsymbol{2}}{\cos(\boldsymbol{\theta_1})} \cos^2(\boldsymbol{k_0 h} \cos(\boldsymbol{\theta_1})). \tag{10}$$

This design equation describes which height *h* of the magnetic dipoles has to be chosen above the ground plane to fully redirect light at normal incidence to the ± 1 diffraction orders.

2. Analytical antenna theory

To implement the metagrating theory into an analytical design structure, we use a method common in antenna theory, and derive the radiation of the total array of magnetic dipoles by summing up the far fields of all individual dipoles. Here, interaction of the dipoles is not taken into account. The far-field radiation by antennas for a magnetic dipole pointing in *x* direction is given by [2]:

$$\mathrm{E_\theta} = \mathrm{i}\omega\eta \frac{\epsilon\, m_x}{4\pi\, \mathrm{r}}\, \mathrm{e}^{-\mathrm{ikr}\, \sin\varphi} \quad , \tag{11}$$

$$\mathrm{E_\varphi} = \mathrm{i}\omega\eta \frac{\epsilon\, m_x}{4\pi\, \mathrm{r}}\, \mathrm{e}^{-\mathrm{ikr}\, \cos\theta \cos\varphi} \tag{12}$$

with φ and θ the azimuthal and zenithal angles, respectively. If we consider a 1D geometry (dipoles in a line), $\varphi = \frac{\pi}{2}$, and the electrical field is described by:

$$\mathbf{E_\theta} = \mathbf{i\omega\eta} \frac{\boldsymbol{\epsilon\, m_x}}{\mathbf{4\pi\, r}}\ \mathbf{e^{-ikr}}. \tag{13}$$

Here, ω is the angular frequency, ε the permittivity, and η the permeability ($k_0 = \omega\eta\epsilon$) and m_x is the magnetic moment which takes the form $m_x = \frac{1}{i\omega} S E_0$ due to the condition $E_0 = Q_0$. If the dipole is located above a ground plane with distance *h*, image theory can be used to describe the far field:

$$\mathbf{E_\theta} = \mathbf{E_\theta^+} + \mathbf{E_\theta^-} = \mathbf{ik_0}\boldsymbol{m_x}\left(\frac{\mathbf{1}}{\mathbf{4\pi\, r^+}}\ \mathbf{e^{-ikr^+}} + \frac{\mathbf{1}}{\mathbf{4\pi\, r^-}}\ \mathbf{e^{-ikr^-}}\right) \tag{14}$$

with r^+ and r^- describing the distance to the dipole located above the ground plane and the image dipole below the ground plane. To calculate the fields in cartesian coordinates r^+ and r^- can be expressed as $r^+ = \sqrt{y^2 + (z-h)^2}$ and $r^- = \sqrt{y^2 + (z+h)^2}$. The far field radiation of N_1 dipoles located next to each other at a distance d_1 (on the y axis) is then given by the sum of all individual dipoles and their image dipole:

$$\boldsymbol{E_{\theta,N_1}} = \sum_{n=0}^{N_1} \boldsymbol{E_\theta^+}(\boldsymbol{y} - \boldsymbol{nd_1}, \boldsymbol{z} - \boldsymbol{h_1}) + \boldsymbol{E_\theta^-}(\boldsymbol{y} - \boldsymbol{nd_1}, \boldsymbol{z} + \boldsymbol{h_1}). \tag{15}$$

Continuing summing of radiated far fields, results in a total far field of all dipoles:

$$\boldsymbol{E_{\theta,tot}} = \sum_{i=0}^{m} \boldsymbol{E_{\theta,N_i}}. \tag{16}$$

of $N = N_1 + N_2 + \ldots + N_m$ dipoles with N_1 dipoles with the distance d_1, N_2 dipoles with the distance d_2 and so on.

Based on this derivation, not taking into account the interaction between particles, a design of the far-field scattering of arrays of magnetic dipoles can be made. It should be noted that the scattering towards 0 degree cannot be canceled mathematically, as here we are considering a finite array, while the design equation (10) is based on an infinite plane wave. For this reason, the analytical calculation gives us information about the overall shape of the angular scattering distribution, but not about its efficiency. Figure S1 shows the analytically calculated far field for the large-angle reflector metasurface, consisting of 5 magnetic dipoles per metagrating, with optimum height derived from the design equation.

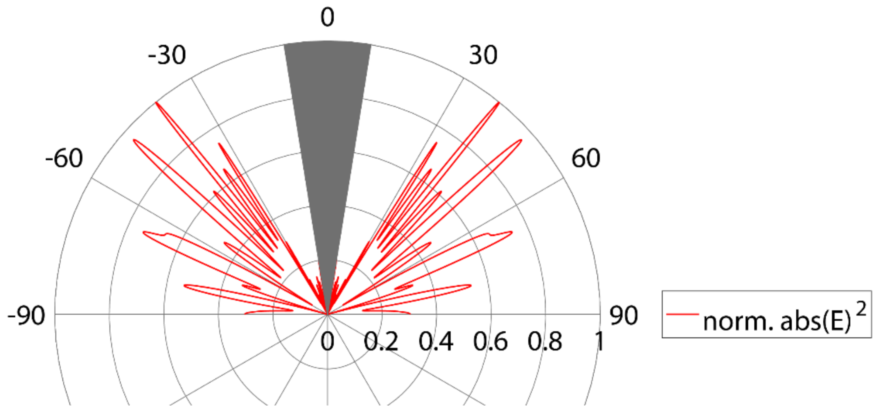

Figure S1 Angular profile of far-field intensity analytically calculated from the sum of 25 point dipoles (5 dipoles per angle, 35-75°) and their image dipoles with their respective distances z each obtained from the design equation. The 0^{th} order scattering contribution is removed (grey zone).

3. Optimization of structure by simulations

In the following steps, it is shown how we designed the final structure for fabrication. In all steps FDTD Lumerical is used. In all simulations for optimization, periodic boundary conditions were used and metagratings with one fixed period were studies. The structure was illuminated with a plane wave and the power to different grating orders was determined using the grating projection functionality of FDTD Lumerical. We choose to optimize the structure for an operational wavelength of λ=650 nm, normally incident on a 1D array of Si pillars placed on a Ag substrate with a silica spacing layer. The array has a period of 919 nm (θ_{diff}=45°). We fix the height *z* of the pillar to 180 nm. Now, by varying the width *w* and the distance h between Ag substrate and center of the pillar, we find that at for *h*=200 nm and w=85 nm, almost 50 % of the reflected light is scattered towards the $+1^{st}$ order, which given the symmetry, translates to almost 100% diffraction efficiency into the n=$\pm$1 modes (Figure S2).

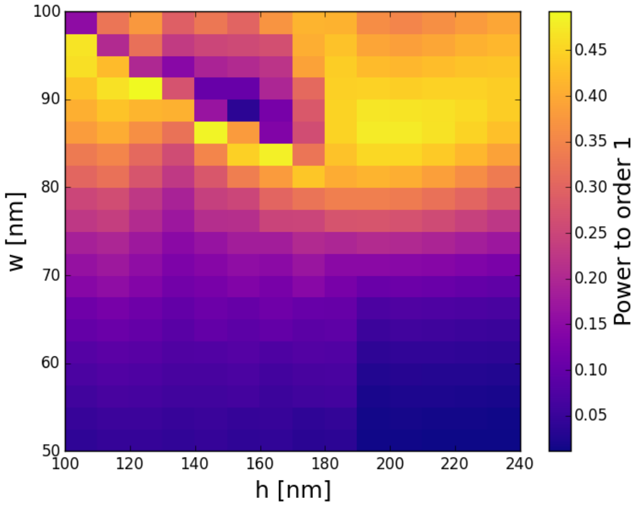

Figure S2 Diffraction efficiency into the 1st diffraction order as a function of distance h from particle to the Ag mirror and particle width w.

For ease of fabrication, the distance *h* was kept constant for all combined metagratings. To investigate the metagrating performance for λ=650 with periodicities different from 919 nm, we vary the period *p* as well as the distance *h* (Figure S3). We find that for *h*=200 nm for the smaller and bigger periods, up to a pitch of p=1300 nm (above which the 2nd diffraction order appears) the grating efficiency can be designed to be above 35% (70% for both n=±1 orders).

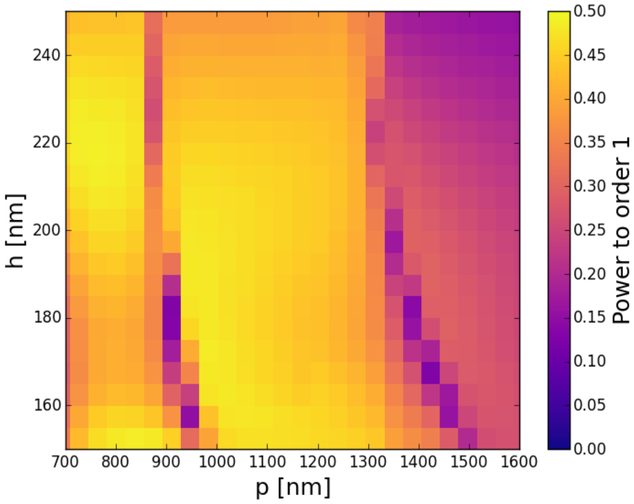

Figure S3 Diffraction efficiency into the 1st diffraction order as a function of array period p and distance h from particle to the Ag mirror.

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In fabrication, the width of the individual metagratings can be easily tailored. We investigate how the width of the individual particles affects the performance for different periodicities and find that w=85 nm gives the best result for all periods (Figure S4).

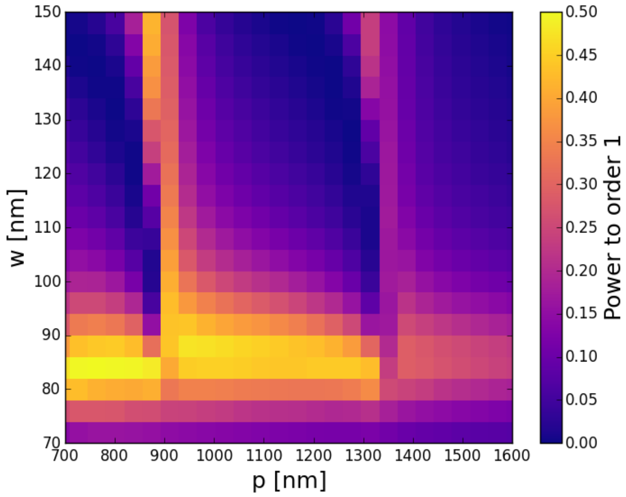

Figure S4 Diffraction efficiency into the 1st diffraction order as a function of array period p and particle width w.

With the chosen parameters (w = 85 nm, z = 180 nm, h = 200 nm), we investigate the effect of varying the array period for the 500-1200 nm spectral range (Figure S5). The resonant scattering effect around 650 nm is clearly seen for all periods, and a high coupling efficiency is observed for the bandwidth of the magnetic Mie mode, peaking near 100% on resonance.

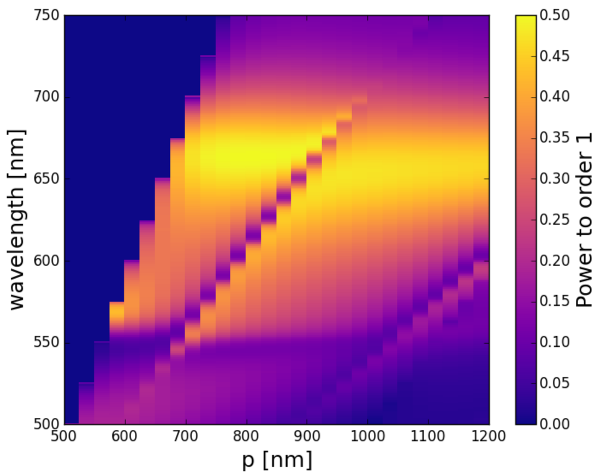

Figure S5 Diffraction efficiency into the 1st diffraction order as a function of array period p and wavelength, showing resonant behavior around 650 nm. No diffraction is observed in the dark blue region.

As described in the main text, for first-order scattering angles $\theta_{diff} < 30°$ higher-order diffraction complicates the design, that focus on optimizing only the ± 1 Floquet modes. As mentioned, we address this problem by modifying the unit cell to contain a number of identical scatterers (3 or 6, depending on the grating pitch) such that their scattering radiation profiles remain within the angular range below 30°. We tune the distance between the scatterers to optimize the scattering profile for the highest coupling efficiency towards the first diffraction order. For coupling to the 5°, 15° and 25° angles, we reach efficiencies between 38% and 48% (76% and 96% for both orders) by choosing optimized inter-particle distances of d = 550 nm, 470 nm and 230 nm, respectively (Figure S6).

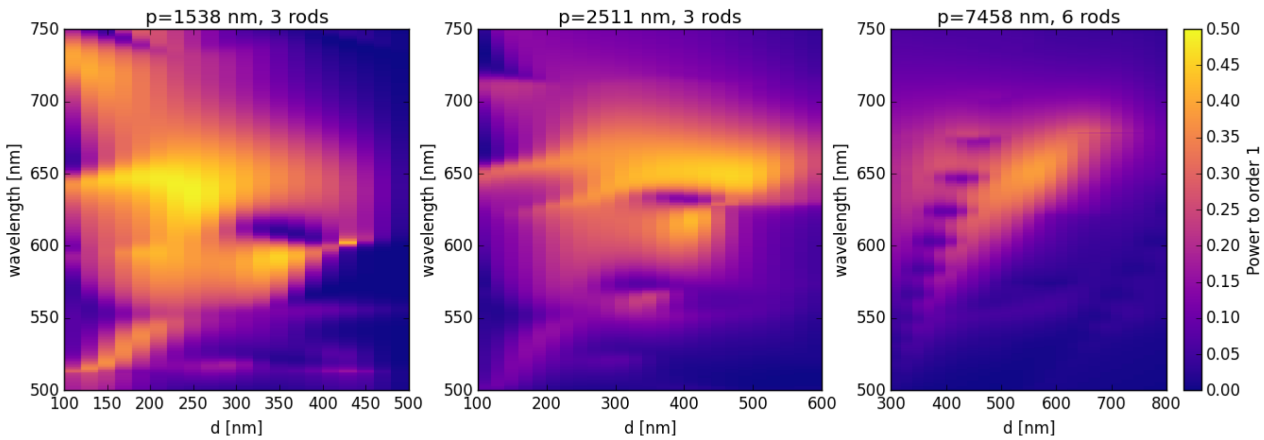

Figure S6 Diffraction efficiency into the 1st diffraction order as a function of Si pillar distance d and wavelength for (a) 3 pillars for θ=25° (b) 3 pillars for θ=15° (c) 6 pillars for θ=5°.

References

[1] Y. Ra'di, D. L. Sounas, and A. Alù, "Metagratings: Beyond the Limits of Graded Metasurfaces for Wave Front Control," *Phys. Rev. Lett.*, vol. 119, no. 6, p. 067404, Aug. 2017.

[2] C. Balanis, *Antenna theory; analysis and design*, vol. 72, no. 7. 1984.