Supplemental Document

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High-efficiency, polarization-insensitive 1400-lines/mm retroreflective metagrating with cascaded nano-optical modes: supplement

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1. SIMULATIONS

The one-dimensional grating and metagrating with cascaded cells are G_0 and G_1G_2, where the material of cells G_0 and G_1G_2 are set to hafnium oxide (HfO_2, $n_G = 2.01$) due to the high index and broad bandgap. The high reflection (HR) films is S(HL)^{17}BA, where S denotes a K9 glass substrate, H and B denote the high-index (Ta_2O_5, $n_H = 2.16$) HR films layers, L and A denote the low-index (SiO_2, $n_L = 1.47$) HR films layers, respectively. The indices of tantalum oxide (Ta_2O_5) and silicon oxide (SiO_2) are experimentally obtained using a spectrograph, and the indices of HfO_2 and K9 glass substrate are experimentally measured using ellipsometry. The -1st order diffraction efficiency (DE) for TE and TM polarizations of one-dimensional grating and metagrating with cascaded cells on the HR films is calculated using rigorous coupled-wave analysis (RCWA). Here, the harmonic number is set to be 5, the incident angle is set to be 48.3° and the incident spectral range is set to be 1040 nm-1090 nm. The particle swarm optimization algorithm (PSO) is used to optimize the parameters of the one-dimensional grating, metagrating with cascaded cells, and HR films. For one-dimensional grating and corresponding HR films, the optimized duty cycle and height range of cell (f_0,h_0) are set as 0.5-0.6 and 400 nm-600 nm, the optimized thickness ranges of HR films (h_A,h_B,h_L,h_H) are set as 100 nm- 250 nm, 100 nm- 250 nm, 150 nm- 250 nm and 100 nm- 200 nm, respectively. For metagrating with cascaded cells and corresponding HR films, the optimized duty cycle and height range of cascaded cells (f_1,f_2,h_1,h_2) are set as 0.35-0.48, 0.6-0.7, 250 nm-350 nm and 250 nm-350 nm. The optimized thickness ranges of HR films (h_A,h_B,h_L,h_H) are set as 100 nm-250 nm, 100 nm-250 nm, 150 nm-250 nm and 100 nm-200 nm, respectively. The merit function (MF) considering -1st broadband DE from 1040 nm to 1090 nm for TE and TM polarizations is set as:

$$\mathrm{MF} = 1 - \min\left\{DE^{TE}_{-1R}(\lambda_1), DE^{TM}_{-1R}(\lambda_1), \cdots, DE^{TE}_{-1R}(\lambda_N), DE^{TM}_{-1R}(\lambda_N)\right\} \tag{S1}$$

Where the wavelength interval ($\lambda_{i+1} - \lambda_i$) of the spectra is 5 nm, N is the number of wavelength discrete points, $DE_{-1R}(\lambda_i)$ is the -1st order DE in the wavelength λ_i.

The optimal results of one-dimensional grating, metagrating with cascaded cells, and their corresponding HR films are presented in Table S1.

We set the variable number of (HL) layers as n. To demonstrate that the number of (HL) layers is 17, we calculated -1st order broadband minimum efficiency from 1040 nm to 1090 nm with n, as shown in Fig. S1. When n is less than 16, -1st order broadband minimum efficiency will decrease, especially for TM-polarization. Therefore, n = 17 is necessary for keeping high diffraction efficiency.

We calculated the diffraction efficiency of optimized metagrating with cascaded cells on the ideal lossless metallic film and HR films, as shown in Fig. S2. The refraction index of the ideal lossless metallic film was set as $n = +\infty$, and the thickness of the ideal lossless metallic film was set at 1um. Similar to the HR layer, the ideal lossless metallic film also offers nearly 100% reflectance. However, the TE-polarization diffraction efficiency of the ideal lossless metallic film is less than 60%, demonstrating that HR films have the advantage of regulating the diffraction efficiency.

Table S1. Compositions and optimized parameters of one-dimensional grating, metagrating with cascaded cells and their corresponding HR films.

Symbol	One-dimensional grating	Metagrating with cascaded cells
Period (nm)	714[p]	714[p]
Duty cycle	0.51[f_0]	0.45[f_1]
		0.61[f_2]
Height (nm)	569[h_0]	290[h_1]
		270[h_2]
HR films (nm)	160[h_A]	165[h_A]
	158[h_B]	135[h_B]
	192[h_L]	192[h_L]
	149[h_H]	149[h_H]

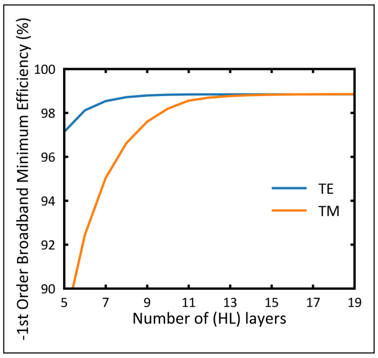

Fig. S1. Calculation results between the number n of (HL) layers and -1st order broadband minimum efficiency.

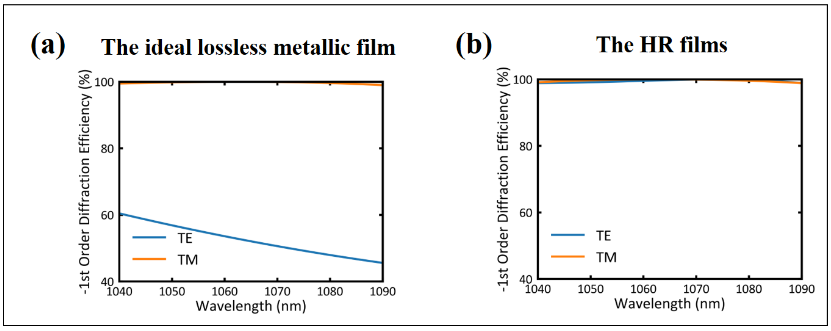

Fig. S2. The -1st order diffraction efficiency of metagrating with cascaded cells on (a) the ideal lossless metallic film and (b) the HR films.

2. ANALYSIS OF MERGED-PARAMETER FABRICATION TOLERANCE

Compared with one-dimensional grating, the metagrating with cascaded cells has more parameters affecting the -1st order DE. Therefore, an evaluation process of merge-parameter fabrication tolerance is designed using the Monte Carlo method. Two main parameters are defined in the tolerance evaluation: allowed range (AR) and qualified value (QV)[1]. The AR of one-dimensional grating with the height (h_0) and width ($f_0 p$) are set as ± 30 nm and ± 20 nm, and the AR of cascaded metagrating with height ($h_1 + h_2$) and width ($f_1 p$, $f_2 p$) are also set as ± 30 nm and ± 20 nm. That is to say, the height and width of one-dimensional grating and metagrating with cascaded cells change in 60 nm and 40 nm total range away from the designed values in a normal distribution. The QV is set to be the -1st order minimum DE over 95% from 1040 nm to 1090 nm. According to the definition of QV, it is known that the bigger the QV is, the larger the fabrication tolerance of the cell can be fabricated.

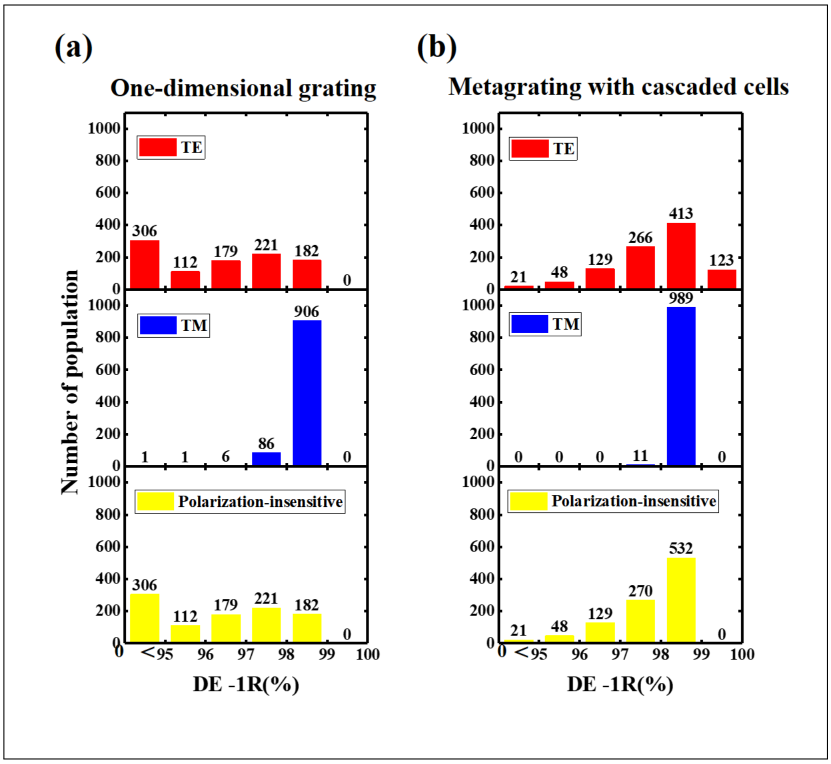

Fig. S3. Calculation of -1st order diffraction efficiency during population size of the designed one-dimensional grating and metagrating with cascaded cells.

When the polarizations of incident light are TE, TM, and polarization-insensitive, respectively, the QV of the one-dimensional grating is 70.4%, 100%, and 70.4%, and the QV of metagrating with cascaded cells is 97.9%, 100%, and 97.9%, which are shown in Figure S3. Based on the evaluation process results, the fabrication of metagrating with cascaded cells is considered to be much easier than one-dimensional grating because of its larger QV.

3. FABRICATION

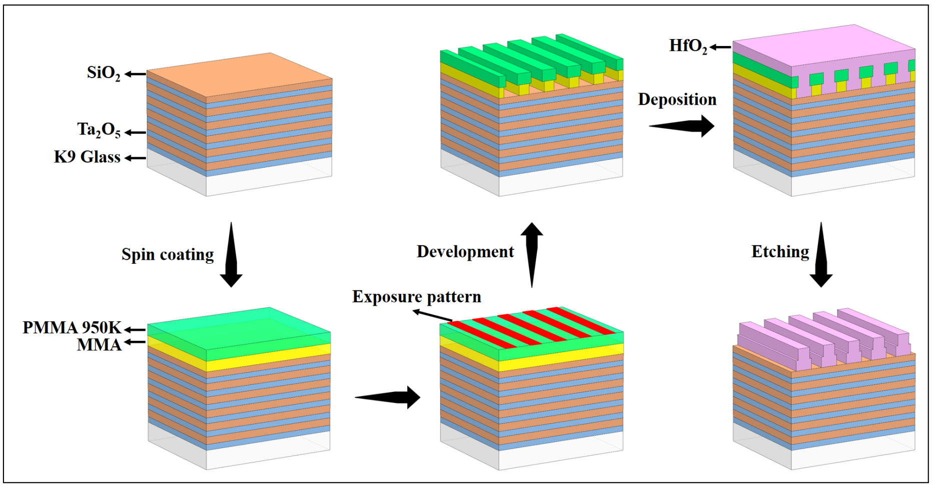

Fig. S4. Illustration of the major fabrication steps of metagrating with cascaded cells on the HR films. (i) HR films are deposited on a K9 glass substrate; (ii) MMA and PMMA 950K are spin-coated onto the HR films; (iii) MMA and PMMA 950K are written on exposure pattern; (iv) T-type photoresist is obtained after development; (v) HfO_2 is coated on T-type photoresist; (vi) The top HfO_2 layer and T-type photoresist are removed.

The HR films of dielectric multilayers is deposited on one-inch round K9 glass substrates using ion-beam assisted deposition in an optorun OTFC-1300 vacuum coating system[2–4]. The deposition rates of SiO_2 and Ta_2O_5 are 8.0 Å/s and 3.0 Å/s respectively. A 270 nm thick Methylmethacrylate (MMA) layer and a 340 nm thick Polymethyl Methactylate (PMMA 950K) are orderly spin-coated on the HR films at 1000 rpm and 1600 rpm respectively. These two-layer photoresists are then baked at 180°C for 10 minutes. A 10 nm thick chromium layer acting as a conductive layer is deposited using thermal evaporation. The exposure pattern is written by e-beam lithography (EBPG5200, Raith) system, the patterning process is carried out at 100 kV using a 10 nm aperture beam current of 2 nA and the exposure dose is 430 μC/cm^2. Subsequently, the sample is developed in a mixed solution of Methyl Isobutyl Ketone (MIBK) and Isopropanol (IPA) (mixed ratio 1:3) at 23 °C. Because the MMA owns higher sensitivity than PMMA950K, the development width of the MMA layer is larger, thus the cascaded trenches with different widths are obtained[5]. The width of the bottom and top trench is 430 nm and 320 nm respectively. A 270 nm thick HfO_2 films deposited by the Atomic Layer Deposition (ALD) technique filled the cascaded stenches due to the conformality of the ALD process[6]. Tetrakis (dimethylamino) Hafnium (TDMAH) and H_2O are chosen as Hf precursor and oxidant, respectively. They could maintain chemical reactions to grow the HfO_2 films at a low deposition temperature of 105 °C. The deposition temperature is lower than the glass transition temperature of MMA and PMMA950K in order to preserve the physical integrity of the photoresist. The HfO_2 deposition rate is almost 0.14 nm/cycle.

Inductively coupled plasma (ICP-RIE) etching[7] with a mixture of CF4 and Ar is applied to etch the HfO_2 layer on the photoresist. The flow rates of CF4 and Ar gas, working pressure, ICP power, RF power, and temperature are maintained at 20 sccm, 80 sccm, 20 mtorr, 150 W and 20 °C, respectively. The etch rate of the HfO_2 layer on the photoresist was about 2.2 Å/s, while the etch rate of the T-type cascaded photoresist is almost 20 Å/s under this condition. It is important to mention that the etching rate of the cascaded photoresist is much higher 10 times than the etching rate of HfO_2 films, which means that the SiO_2 match layer under the photoresist is easily over etched. To avoid the fabrication imperfection, the etching parameters and etching times should be carefully adjusted to obtain the metagrating with cascaded cells.

4. THE DIFFRACTION EFFICIENCY OF FABRICATED METAGRATING WITH CASCADED CELLS

The diffraction spectrum of the metagrating with cascaded cells is tested by an angle-resolved spectrum system based on Fourier transform from Ideaoptics[8], as shown in Figure S5a. The scatter diagram is shown in Figure S5b. The -1st order DE of the fabricated metagrating with cascaded cells is measured at the incidence angle of 48.3° for TE polarization and TM polarization. The measured wavelength range is from 1040 nm to 1090 nm, and the diffraction angle range is from 45.3° to 51.4°. The intensity of incident light was detected via the Ag mirror. Then, the intensities of -1st and 0th order diffraction lights were detected to obtain the -1st diffraction efficiency. Testing was carried out in a darkroom under air environment. The scatter diagram is fitted based on the least square method and the simulated data is calculated based on fabricated metagrating parameter with cascaded cells, as shown in Figure S5c. In this study, the fitted -1st order DE exceeds 96% in a 50 nm-wide-wavelength range, which is similar to the simulation result of the fabricated metagrating with cascaded cells.

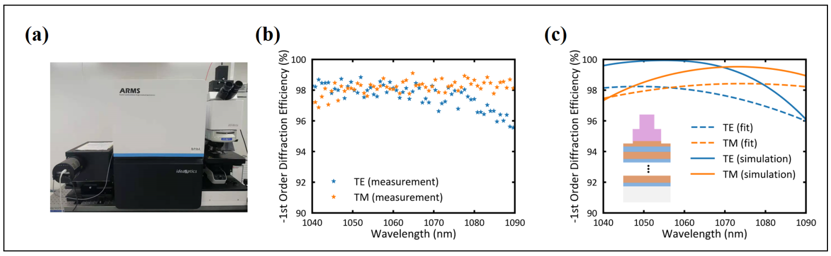

Fig. S5. (a) The angle-resolved spectrum system. (b) Measured scatter diagram of -1st order diffraction spectra. (c) Fitting diagram of measured scatter data and simulated diagram of fabricated metagrating with cascaded cells.

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