Supplementary Information

Computational hyperspectral devices based on quasi-random metasurface supercells

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Part 1: Principle of the spectral reconstruction algorithm.

According to Eq. (1) of this study, the compressive sensing algorithm based on sparse optimization and dictionary learning ^{1,2} has been used to reconstruct the incident spectral signal. A sparse incident signal is an essential prerequisite for realizing compressed sensing is the sparse incident signal. However, since most spectra are not sparse in natural environments, the incident spectral signals need to be sparsely processed and represented as follows:

$$f = \Psi s$$
 (S1)

where, f represents an incident spectrum. Ψ and s represent the sparse basis matrix and sparse coefficient, respectively. Thus, Eq. (1) can be rewritten as follows:

$$I = T\Psi s \tag{S2}$$

where I and T represent the observation signal and observation matrix of the compressive sensing algorithm, respectively. Based on Eq. (S2), the problem of solving the incident signal can be converted into the l_1 norm as follows:

$$\min \|s\|_{1} \quad \text{s.t.} \quad \|f\Psi s - I\|_{2} \le \delta \tag{S3}$$

$$\left\|s\right\|_{1} = \sum_{j=1}^{m} f_{j} \tag{S4}$$

where, δ represents a positive constant. The optimal solution *s* for Eq. (S3) and Eq. (S4) can be obtained simultaneously. The incident spectrum *f* can be calculated according to Eq. (S1). Presently, many algorithms for solving the original signal based on the given principle.³ The orthogonal matching pursuit (OMP) algorithm has been used to reconstruct the spectral signal in this work due to its high optimization efficiency. The pseudo-code of OMP is given as follows:

- (1) Input: $y=T^*f$, $A=T^*\Psi$, sparsity = k;
- (2) Initialization: residual r=y, define two empty matrices (AA and PP);
- (3) Computation: [val, pos]=max($A^{T*}r$), $AA_i = [AA_{i-1}, A(:, pos)]$, $PP_i = [PP_{i-1}, pos]$, $X = (AA^{T*}AA)^{-1*}A^{T*}r$;
- (4) Update residual: r=y-AA*X;
- (5) Judgment: i=i+1, if i < k, return to step (3);
- (6) Output: reconstructed original signal $f'=\Psi^*X$.

Part2: Metasurface fabrication



Fig. S1 The fabrication process of the samples

A 200 nm Si film was epitaxially grown on the Al₂O₃ substrate. Then, an electron beam photoresist was spin-coated on the Si film. Next, a quasi-random metasurface supercell array pattern was displayed on the photoresist using electron beam lithography (EBL), which was transferred onto the Si film by inductively coupled plasma (ICP). Finally, the photoresist is removed, completing the processing of the samples.

Part 3: Schematic representation of quasi-random metasurface supercells selected by the optimization algorithm.

T81_1	T81_2	T81_3	T81_4	181_5	181_6	10 T81_7	T81_8	O T81_9
0 T81_10	к х Ц у Т81_11	T81_12	T81_13	T81_14	T81_15	T81_16	T81_17	T81_18
T81_19	T81_20	T81_21	••• ••• T81_22	T81_23	T81_24	T81_25	T81_26	T81_27
T81_28	10 T81_29	T81_30	T81_31	T81_32	T81_33	T81_34	T81_35	T81_36
T81_37	T81_38	T81_39	T81_40	T81_41	T81_42	T81_43	T81_44	8 T81_45
T81_46	T81_47	T81_48	781_49	T81_50	T81_51	T81_52	T81_53	10 T81_54
101 T81_55	T81_56	T81_57	T81_58	181_59	T81_60	T81_61	T81_62	T81_63
T81_64	E T81_65	T81_66	T81_67	T81_68	T81_69	T81_70	181_71	T81_72
T 81_73	T81_74	T81_75	T81_76	T81_77	T81_78	T81_79	T81_80	T81_81
			Si			Al ₂ O ₃		

Fig. S2 The top views of the 81 quasi-random metasurface supercells selected by the optimization algorithm.



Fig. S3 The top views of the 49 quasi-random metasurface supercells selected by the optimization algorithm.





Fig. S4. Transmission spectra obtained by the simulation of the metasurface supercells shown in Fig. S1.



Fig. S5. Transmission spectra obtained by the simulation of the metasurface supercells shown in Fig. S2.





Fig. S6 Transmission spectra obtained by the simulation of 36 metasurface cells for a previously reported study.⁴ The geometric parameters of the metasurface cells as per the referred study.⁴ The simulation conditions and materials are consistent with those



Fig. S7 Pearson's correlation coefficient of the 36 transmission spectra shown in Fig. S5. The black dotted line is the average values of Pearson's correlation coefficients.



Part 6: Simulation results of the complex narrowband spectral reconstruction.

Fig. S8 Simulation results of narrowband spectrum reconstructed by the CHDBS consists of 49 metasurface supercells (n=49). The incident spectra in (a), (b), (c), and (d) correspond to the incident spectra given in Figs. 4(a), (f), (g), and (h), respectively.



Part 7: Experimental results of the metasurface supercell arrays.

Fig. S9 Experimentally measured transmission spectra of the metasurface supercells shown in Fig. S1.



Fig. S10 Experimentally measured transmission spectra of the metasurface supercells shown in Fig. S2.

References

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