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:

$$
f=\Psi_S \tag{S1}
$$

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:

$$
\min \|s\|_1 \quad \text{s.t.} \quad \|f\Psi s - I\|_2 \le \delta \tag{S3}
$$

$$
\|s\|_{1} = \sum_{j=1}^{m} f_{j}
$$
 (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 $i \leq k$, return to step (3);
- (6) Output: reconstructed original signal *f'*=Ψ**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	$T81_3$	$T81_4$	$T81_5$	T81_6	T81_7	$T81_8$	T81_9
T81_10	T81_11	T81_12	$T81_13$	$T81_14$. TITE e d'Arre T81_15	T81_16	$T81_17$	バロッ $T81_18$
$T81_19$	T81_20	a matsa EO I VIII A T81_21	$\phi \cdot \phi$. T81_22	T81_23	T81_24	T81_25	T81_26	T81_27
T81_28	T81_29	\mathbf{u} T81_30	T81_31	T81_32	T81_33	T81_34	T81_35	T81_36
T81 37	T81 38	T81 39	T81 40	SL 69 T81 41	T81 42	T81 43	T81 44	T81 45
71 IX T81_46	6 F T81_47	T81_48	к. 21 W T81_49	T81 50	T81_51	61 N T81_52	T81_53	T81_54
T81_55	T81_56	T81_57	o Sa T81_58	T81_59	T81_60	T81_61	5 H H W T81 62	T81_63
T81_64	T81_65	T81_66	T81_67	T81_68	T81_69	T81_70	T81_71	وبعره T81_72
T81 73	ı. T81 74	T81 75	w T81_76	T81 77	T81_78	T81_79	T81 80	T81 81
			Si			Al_2O_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.

Part 4: Simulation results of the metasurface supercells.

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

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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