Supporting Information

Efficient inverse design of optical multilayer nano-thin films using neural network principles: backpropagation and gradient descent

Jun Hee Han[*a]

a. School of Electrical Engineering, the Korea Advanced Institute of Science and Technology, Yuseong-gu, Daejeon 34141, Republic of Korea

1. Inverse Design

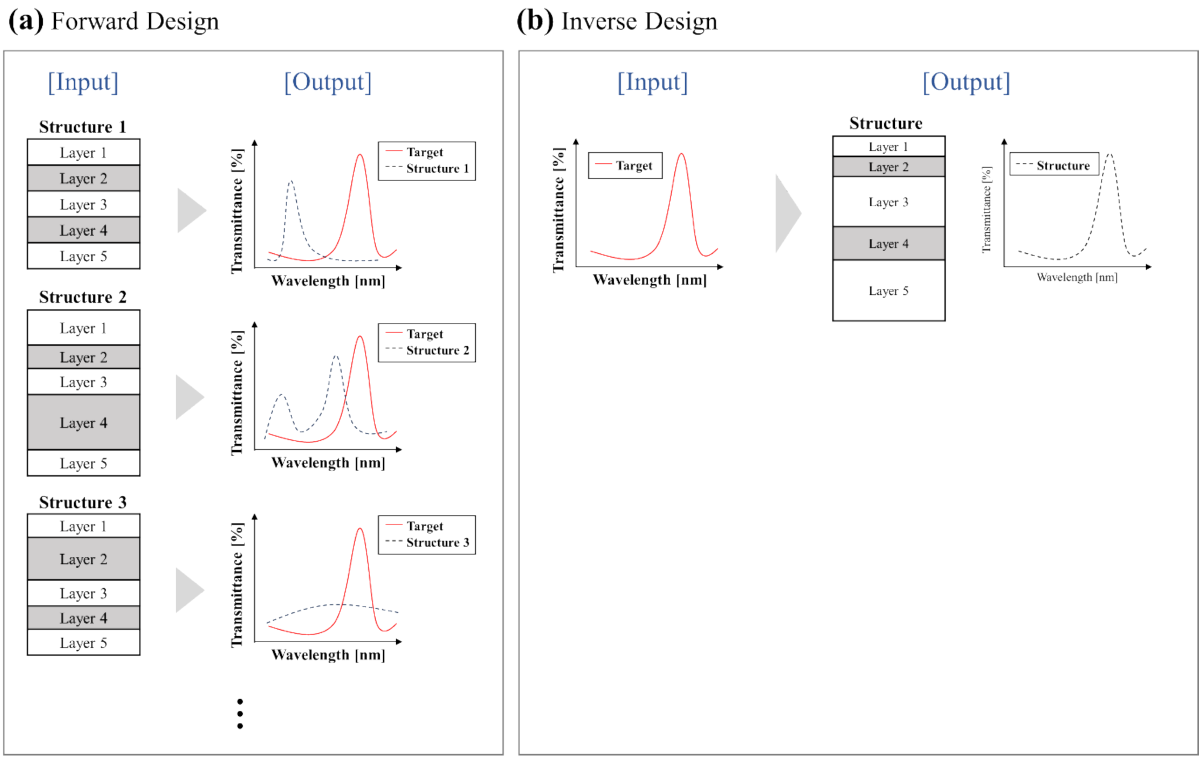

Figure S1. Two methods to design a nano thin film with specific optical properties. (a) Forward Design: In this approach, a film structure is initially specified. The optical properties of the structure are then determined, and the process is iterated until the desired optical property is achieved. (b) Inverse Design: In this method, the desired optical property is specified first. A structure that can realize this property is then derived.

In previous approaches, optical design involved an iterative process of specifying the device structure and subsequently evaluating its optical properties. Initially, various candidate structures were determined, and their optical properties were individually assessed to identify a structure that met the desired optical criteria. This methodology is known as "forward design" (Fig S1a.) Recently, a new method called "inverse design" that utilizes neural networks has been studied. Unlike forward design, inverse design begins by specifying the desired optical property. Once the target property is defined, the inverse design method generates a candidate structure that can achieve this property. This approach significantly shortens the design process and reduces the time required compared to the forward design method (Fig S1b)[1].

2. Introduction of artificial neural networks

Neuron and perceptron

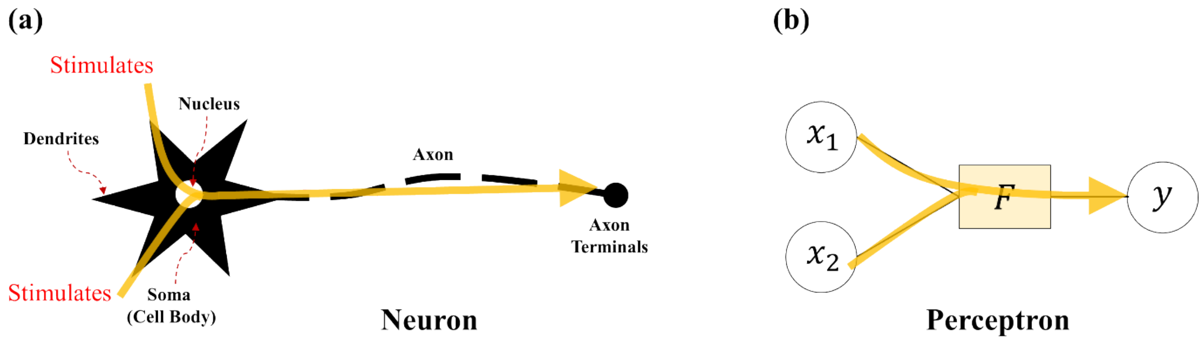

Figure S2. Basic building blocks of a neural network. (a) The basic unit of the brain is the neuron. (b) The basic unit of an artificial neural network is the perceptron, modeled after the neuron.

The human brain consists of nerve cells called neurons (Figure S2a)[2]. A neuron's structure is divided into dendrites, which receive external stimuli, a cell body that processes these signals, and an axon that transmits the processed signals to other neurons via the axon terminal. Artificial neural networks are modeled after this structure, with perceptrons serving as the basic units, functioning similarly to neurons (Figure S2b)[3]. Like a neuron receiving external stimuli, a perceptron receives values from the previous perceptron. These values are processed based on the perceptron's functions, akin to signal processing in the cell body, and the processed value is then transmitted to the next perceptron.

Forward propagation, weight & bias

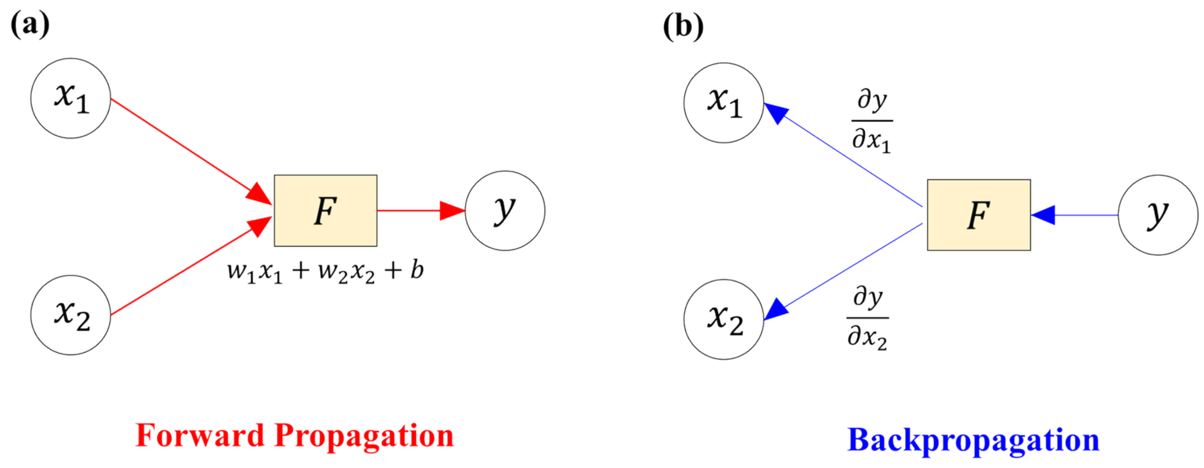

Figure S3. Presentation of forward propagation and backpropagation. (a) Forward propagation refers to the process where input values are computed in each perceptron to produce the output. (b) Backpropagation is the process of computing from the output back to the input values to obtain the gradient of each input value relative to the output.

As described earlier, input values are calculated to generate new values, which are then passed to the next perceptron to obtain the final output. This process is called "forward propagation" (Fig S3a). During forward propagation, the input values are multiplied by weights and biases are added. The reason for this process is to assign the appropriate weight to each input value. The process of multiplying each input by its weight and adding a bias is analogous to how human neural networks function. For example, consider a neuron connected to the part of the brain that perceives pain in the skin. If this neuron receives both a nociceptive (pain) signal and an olfactory (smell) signal, it should be more sensitive to the nociceptive signal. This means the nociceptive signal should be weighted more heavily, making the neuron more responsive to it. Similarly, in a perceptron, certain input paths may need to be processed with greater sensitivity, or there may be situations where two input values need to be considered in combination. Therefore, each input value is multiplied by its own weight and a bias is added. In some cases, the signal is processed using a formula that accounts for these complex situations. The formulas that reflect the weights and biases of the perceptrons in the artificial neural network proposed in this paper are given in eq 2 through eq 5 and eq 7 through eq 12 in the main script.

Backpropagation

Backpropagation is a process in which a calculation result is propagated in the opposite direction of forward propagation (Fig S3b)[4]. In this process, the propagated calculation result represents the gradient of the loss function with respect to each input of the perceptron. By backpropagating from the loss function, which is the output of the proposed network, to the layer thickness node, the effect of layer thickness on the loss function can be determined. This allows for inverse design through efficient thickness updates using the gradient. The chain rule is utilized in the backpropagation process. An example of the result of backpropagation using the chain rule can be found in eq 14, eq 19, and eq 20.

3. Single wavelength target & multi-wavelength target inverse design

The artificial neural network proposed in this paper can be utilized for both single-wavelength target inverse design and multi-wavelength target inverse design. Single-wavelength target inverse design refers to finding a device structure that satisfies the target optical property for a specific wavelength. In contrast, multi-wavelength target inverse design involves finding a device structure that meets the target optical property across a specific range of wavelengths.

For single-wavelength target inverse design, it is sufficient to check the optical target corresponding to a specific wavelength. Thus, the values corresponding to the target wavelength can be used for all the parameters required in eq 13 of the main manuscript. In particular, the refractive index and wavenumber, which can vary for different wavelengths, can be calculated using the values specific to the target wavelength to obtain a device structure that satisfies the expected optical properties.

Since multi-wavelength target inverse design must satisfy the optical properties across a range of wavelengths, calculations are performed using a matrix. One advantage of artificial neural networks is their ease of matrix utilization during computations. In inverse design calculations, parameters such as layer thickness, refractive index, and wavenumber are input in matrix form with values corresponding to the targeted wavelength range. For example, if we assume a multi-wavelength target inverse design between 400 nm and 750 nm, the layer thickness can be expressed in matrix form as shown in eq S1. To perform the process shown in Fig. 3 of the main manuscript, the initialized layer thickness is set to have property $t_{400nm} = t_{401nm} = \cdots = t_{750nm}$. Property $t_{400nm} = t_{401nm} = \cdots = t_{750nm}$ indicates that the layer has a uniform thickness, even though it is represented as a matrix. The reason for performing calculations in matrix form is that the refractive index and wavenumber have different values for each wavelength. If an independent inverse design is performed for each wavelength, the optimal thickness value for each wavelength will differ. After inverse design, the matrix obtained with the optimal layer thickness is expressed as equation S2, which may have the characteristics of property $t'_{400nm} \neq t'_{401nm} \neq \cdots = t'_{750nm}$.

$$Init.t_{\lambda} = \begin{bmatrix} t_{400nm} \\ t_{401nm} \\ \vdots \\ t_{750nm} \end{bmatrix} \tag{S1}$$

$$Opt.t_{\lambda} = \begin{bmatrix} t'_{400nm} \\ t'_{401nm} \\ \vdots \\ t'_{750nm} \end{bmatrix} \tag{S2}$$

For example, in the inverse design of the red transmittance optical nano thin film shown in Fig. 4 of the main manuscript, each layer is initialized as shown in equation S3. At this stage, the initial value of each layer can be set randomly. After performing the inverse design process proposed in this paper, starting from eq S3, the result is obtained as eq S4. Different thickness values are achieved for different wavelengths. By checking the optical spectrum with obtained results, eq S4, it is confirmed that the result is designed to realize the target optical property (Fig. S4).

$$Init.t_{1;\lambda} = \begin{bmatrix} 90\ nm \\ 90\ nm \\ \vdots \\ 90\ nm \end{bmatrix}, Init.t_{2;\lambda} = \begin{bmatrix} 7\ nm \\ 7\ nm \\ \vdots \\ 7\ nm \end{bmatrix}, Init.t_{3;\lambda} = \begin{bmatrix} 130\ nm \\ 130\ nm \\ \vdots \\ 130\ nm \end{bmatrix}, Init.t_{4;\lambda} = \begin{bmatrix} 5\ nm \\ 5\ nm \\ \vdots \\ 5\ nm \end{bmatrix}, Init.t_{1;\lambda} = \begin{bmatrix} 246\ nm \\ 246\ nm \\ \vdots \\ 246\ nm \end{bmatrix} \tag{S3}$$

$$Opt.t_{1;\lambda} = \begin{bmatrix} 79\ nm \\ 80\ nm \\ \vdots \\ 66\ nm \end{bmatrix}, Opt.t_{2;\lambda} = \begin{bmatrix} 5\ nm \\ 5\ nm \\ \vdots \\ 3\ nm \end{bmatrix}, Opt.t_{3;\lambda} = \begin{bmatrix} 146\ nm \\ 147\ nm \\ \vdots \\ 105\ nm \end{bmatrix}, Opt.t_{4;\lambda} = \begin{bmatrix} 40\ nm \\ 41 nm \\ \vdots \\ 29\ nm \end{bmatrix}, Opt.t_{1;\lambda} = \begin{bmatrix} 246\ nm \\ 247\ nm \\ \vdots \\ 222\ nm \end{bmatrix} \tag{S4}$$

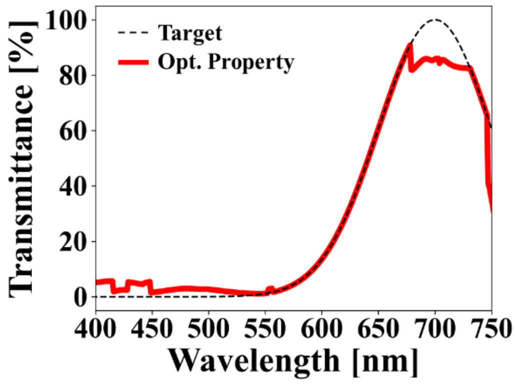

Figure S4. Optical property of nano thin film obtained through inverse design. The black dashed line represents the targeted optical property spectrum. The red solid line shows the optical property of the nano thin film with thickness as eq S4.

However, it is not feasible to have a device with different thicknesses for each wavelength. Therefore, it is necessary to select a representative thickness in the multi-wavelength target inverse design process. The representative thickness is determined by selecting the thickness for each wavelength, checking the optical property, calculating the loss relative to the target property, and choosing the wavelength thickness with the lowest loss value as the representative thickness. For example, in eq S4, the value corresponding to the 575 nm wavelength is $t_1 = 70\ nm, t_2 = 36\ nm, t_3 = 116\ nm, t_4 = 35\ nm, t_5 = 223\ nm$. By configuring the thickness matrix as in eq S5 and checking the optical property and loss, you can obtain the result shown in the Fig. S5a. The results for sets of thicknesses corresponding to the $480\ nm$ and $600\ nm$ wavelengths are shown in Fig. S5b and Fig. S5c, respectively. By performing the same process for all wavelengths within the specified range and checking the loss values, the results was obtained as shown in Fig. S6. In the inverse design of the red transmittance nano thin film, the lowest loss was found in the thickness set corresponding to the wavelength of $600\ nm$. Therefore, the thickness corresponding to $600\ nm$ was selected as the final design result. The selected thickness is indicated in the main manuscript. Although the multi-wavelength target inverse design involves an additional step of selecting a representative thickness, it is much more efficient than the typical forward design, as it narrows down the candidates to a specific number of targeted wavelengths.

$$t_{1;\lambda} = \begin{bmatrix} 70\ nm \\ 70\ nm \\ \vdots \\ 70\ nm \end{bmatrix}, t_{2;\lambda} = \begin{bmatrix} 36\ nm \\ 36\ nm \\ \vdots \\ 36\ nm \end{bmatrix}, t_{3;\lambda} = \begin{bmatrix} 116\ nm \\ 116\ nm \\ \vdots \\ 116\ nm \end{bmatrix}, t_{4;\lambda} = \begin{bmatrix} 35\ nm \\ 35\ nm \\ \vdots \\ 35\ nm \end{bmatrix}, t_{1;\lambda} = \begin{bmatrix} 223\ nm \\ 223\ nm \\ \vdots \\ 223\ nm \end{bmatrix} \quad \text{(S5)}$$

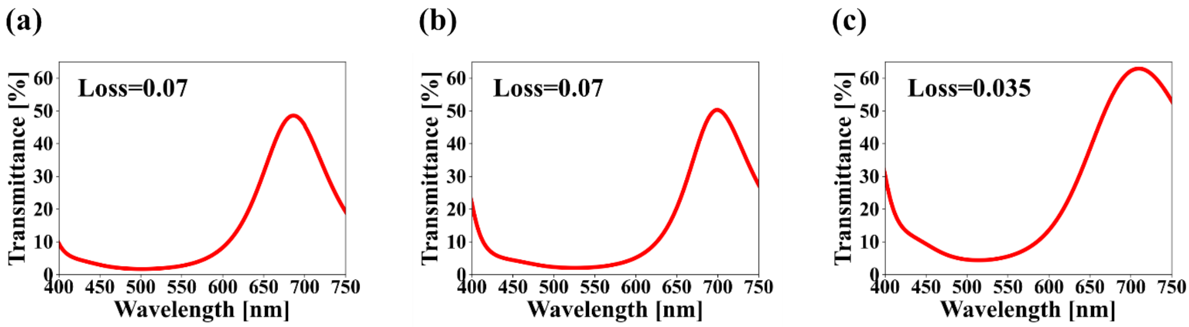

Figure S5. Optical properties of the nano thin film with structures obtained through inverse design. The optical properties were evaluated by selecting a representative thickness from the inverse design results and applying it to the nano thin film. (a), (b), and (c) show the results of applying the thicknesses corresponding to 575 nm, 480 nm, and 600 nm wavelengths as representative thickness, respectively. The mean squared error loss values with respect to the target spectrum are 0.07, 0.07, and 0.035, respectively.

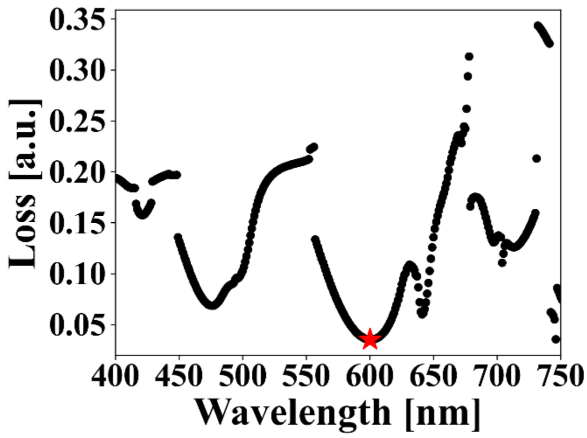

Figure S6. The mean squared error loss value of the optical spectrum relative to the target spectrum when the representative thickness of each layer is selected for the thickness corresponding to a specific wavelength in the optimized layer thickness obtained through inverse design.

4. Multiple local minima

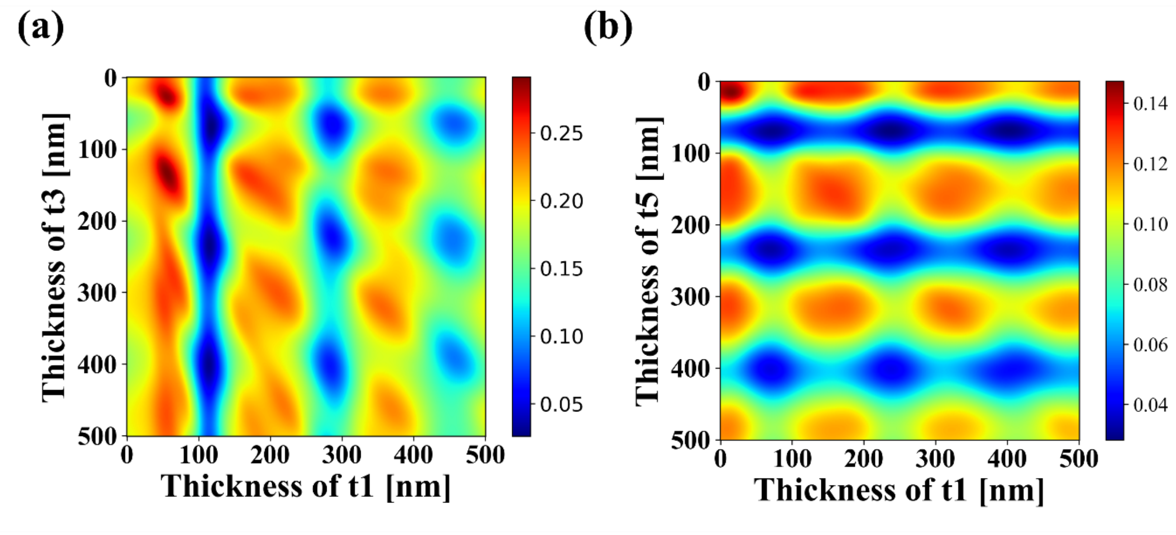

Figure S7. A graph depicting the periodicity of the loss value is presented. (a) Illustrating the loss values concerning t1 and t3, ranging from 0nm to 500nm, respectively. (b) Illustrating the loss values corresponding to t1 and t5, with values ranging from 0nm to 500nm, respectively.

5. Results of extracting ten optimal thicknesses for each color target spectrum

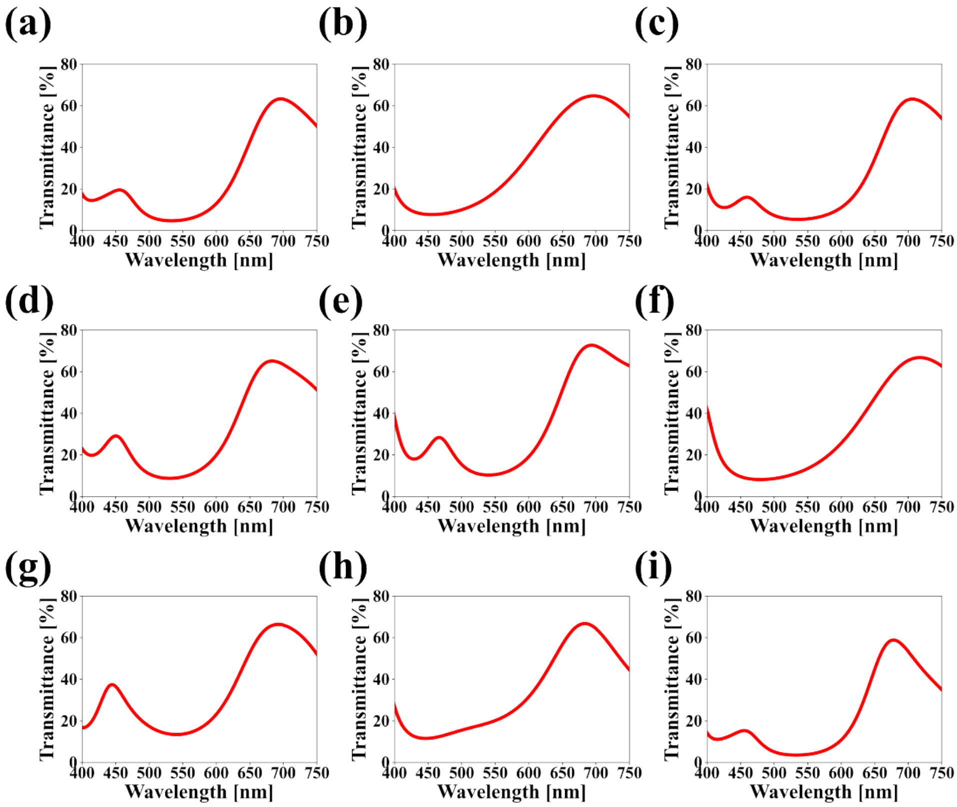

Figure S8. The output spectrum of a thin multilayer film exhibits variations in layer thickness while consistently transmitting only the red region. Each graph corresponds to the thickness values listed in Table S1.

Table S1. The exact thickness of each layer in a red-colored transmissive multilayer thin film of different thicknesses achieved through inverse design.

	t_1	t_2	t_3	t_4	t_5
(a)	242 nm	28 nm	117 nm	25 nm	216 nm
(b)	59 nm	29 nm	117 nm	23 nm	60 nm
(c)	240 nm	30 nm	120 nm	24 nm	63 nm
(d)	234 nm	26 nm	111 nm	19 nm	0 nm
(e)	243 nm	20 nm	122 nm	22 nm	68 nm
(f)	71 nm	23 nm	125 nm	24 nm	58 nm
(g)	228 nm	29 nm	109 nm	12 nm	146 nm
(h)	78 nm	22 nm	112 nm	20 nm	153 m
(i)	241 nm	26 nm	115 nm	32 nm	218 nm

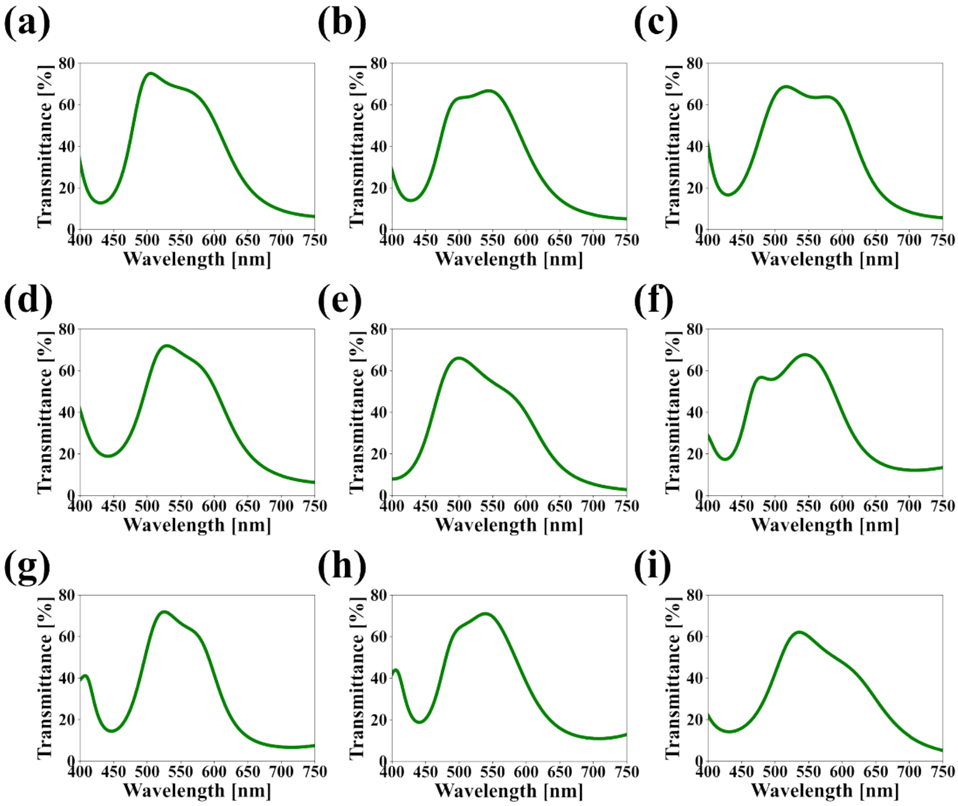

Figure S9. The output spectrum of a thin multilayer film exhibits variations in layer thickness while consistently transmitting only the green region. Each graph corresponds to the thickness values listed in Table S2.

Table S2. The exact thickness of each layer in a green-colored transmissive multilayer thin film of different thicknesses achieved through inverse design.

	t_1	t_2	t_3	t_4	t_5
(a)	168 nm	18 nm	198 nm	17 nm	170 nm
(b)	153 nm	19 nm	200 nm	19 nm	180 nm
(c)	161 nm	19 nm	211 nm	17 nm	150 nm
(d)	170 nm	20 nm	204 nm	18 nm	16 nm
(e)	170 nm	24 nm	72 nm	27 nm	151 nm
(f)	166 nm	23 nm	183 nm	8 nm	280 nm
(g)	291 nm	20 nm	206 nm	17 nm	154 nm
(h)	292 nm	20 nm	192 nm	11 nm	167 nm
(i)	187 nm	26 nm	77 nm	27 nm	33 nm

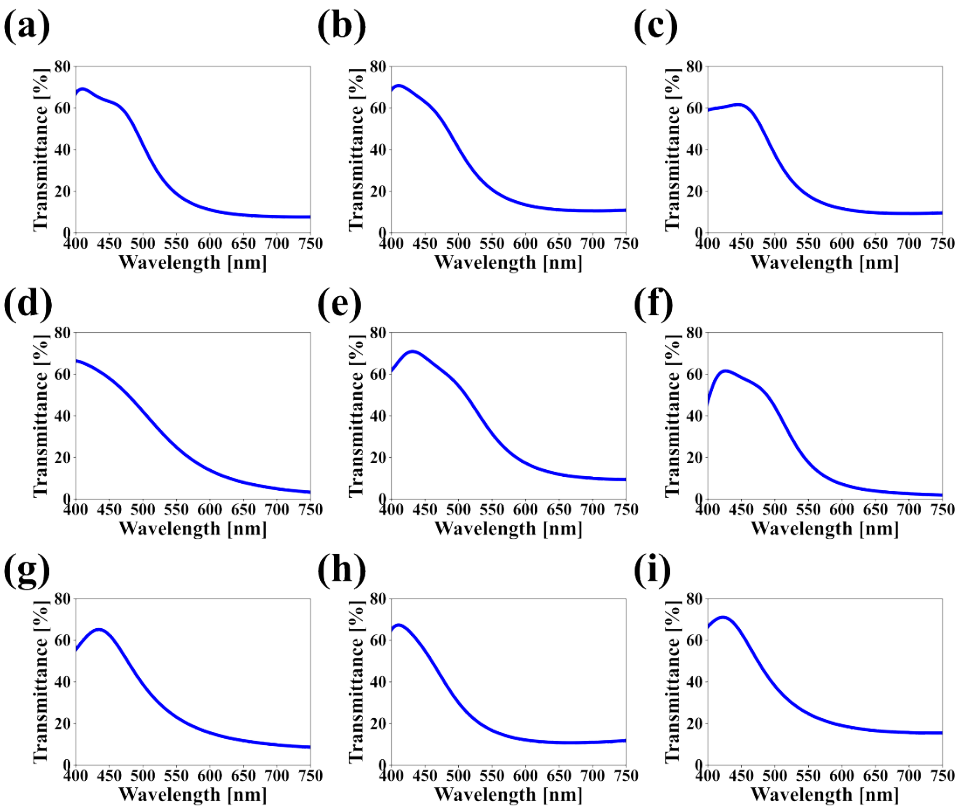

Figure S10. The output spectrum of a thin multilayer film exhibits variations in layer thickness while consistently transmitting only the blue region. Each graph corresponds to the thickness values listed in Table S3.

Table S3. The exact thickness of each layer in a blue-colored transmissive multilayer thin film of different thicknesses achieved through inverse design.

	t_1	t_2	t_3	t_4	t_5
(a)	121nm	23 nm	45 nm	15 nm	95 nm
(b)	114 nm	21 nm	38 nm	11 nm	109 nm
(c)	111 nm	13 nm	36 nm	21 nm	108 nm
(d)	25 nm	30 nm	49 nm	26 nm	33 nm
(e)	122 nm	21 nm	44 nm	12 nm	122 nm
(f)	135 nm	29 nm	51 nm	27 nm	29 nm
(g)	123 nm	25 nm	40 nm	13 nm	31 nm
(h)	110 nm	19 nm	25 nm	13 nm	119 nm
(i)	115 nm	19 nm	20 nm	9 nm	3 nm

References

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