Inverse design and realization of an optical cavity-based displacement transducer with arbitrary response

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Section 1: Theoretical model of reflection in condition of anisotropic media

Regarding the reflection by anisotropic stratified systems, we start from Maxwell’s equations

$$\nabla \times \mathbf{E} = -i\omega\mathbf{B}$$
$$\nabla \times \mathbf{H} = i\omega\mathbf{D}$$ \hspace{1cm} (S1.1) 

Putting the Cartesian components of electromagnetic-field vectors together in a column, we have two column vectors \(\mathbf{I}\) and \(\mathbf{J}\), whose elements are \(E_x, E_y, E_z\), followed by \(H_x, H_y, H_z\), and \(D_x, D_y, D_z\) followed by \(B_x, B_y, B_z\). Then, the matrix form of Eq. (S1.1) can be written as

$$\begin{bmatrix}
0 & 0 & 0 & 0 & -\partial/\partial z & \partial/\partial y \\
0 & 0 & 0 & -\partial/\partial z & 0 & -\partial/\partial x \\
0 & 0 & 0 & -\partial/\partial y & 0 & \partial/\partial x \\
-\partial/\partial z & 0 & \partial/\partial x & 0 & 0 & 0 \\
\partial/\partial y & -\partial/\partial x & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z \\
H_x \\
H_y \\
H_z
\end{bmatrix}
= i\omega
\begin{bmatrix}
D_x \\
D_y \\
D_z \\
B_x \\
B_y \\
B_z
\end{bmatrix}$$

$$\Rightarrow \mathbf{O}\mathbf{I} = i\omega\mathbf{J}.$$ \hspace{1cm} (S1.2)

The constitutive relation between \(\mathbf{I}\) and \(\mathbf{J}\) can be put as the following, in the absence of nonlinear optical effects and dispersion

$$\mathbf{J} = A\mathbf{I},$$ \hspace{1cm} (S1.3)

where \(A\) is the optical matrix, which carries the information about the anisotropic optical properties of the medium

$$A = \begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} & \rho_{11} & \rho_{12} & \rho_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} & \rho_{21} & \rho_{22} & \rho_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} & \rho_{31} & \rho_{32} & \rho_{33} \\
\rho_{11} & \rho_{21} & \rho_{31} & \mu_{11} & \mu_{12} & \mu_{13} \\
\rho_{12} & \rho_{22} & \rho_{32} & \mu_{21} & \mu_{22} & \mu_{23} \\
\rho_{13} & \rho_{23} & \rho_{33} & \mu_{31} & \mu_{32} & \mu_{33}
\end{bmatrix} = \begin{bmatrix}
\varepsilon & \rho \\
\rho' & \mu
\end{bmatrix},$$ \hspace{1cm} (S1.4)

in which \(\varepsilon, \mu, \rho\) are the permittivity, permeability, and optical-rotation tensors. Then Eq. (S1.2) converts to the form as

$$\mathbf{O}\mathbf{I} = i\omega A\mathbf{I}.$$ \hspace{1cm} (S1.5)

Assume that the light is incident from an isotropic ambient medium onto an investigated stratified structure along the positive z-axis, and the coordinate system is shown in Fig. S1. From the symmetry, it is easy to obtain

$$\partial/\partial y = 0.$$ \hspace{1cm} (S1.6)

In addition, it is straightforward to have the spatial dependence along the x-axis since all fields should vary in the x-direction as \(e^{-i\xi x}\)

$$\partial/\partial x = -i\zeta,$$ \hspace{1cm} (S1.7)

where \(\zeta\) can be expressed by the refractive index \(nr_0\) of the ambient and the incident angle \(\varphi_0\),

$$\zeta = \frac{nr_0\sin\varphi_0}{\lambda}.$$ \hspace{1cm} (S1.8)

Substituting Eq. (S1.6) and (S1.7) into Eq. (S1.5), operator \(O\) generates two linear homogeneous algebraic equations and four linear homogeneous first-order differential equations, which means the dimension of Eq. (S1.5) can be reduced to a 4 × 4 matrix form

$$\frac{\partial}{\partial z} \begin{bmatrix}
E_x \\
H_y \\
E_z \\
H_x
\end{bmatrix}
= -i\omega \begin{bmatrix}
\Delta_{11} & \Delta_{12} & \Delta_{13} & \Delta_{14} \\
\Delta_{21} & \Delta_{22} & \Delta_{23} & \Delta_{24} \\
\Delta_{31} & \Delta_{32} & \Delta_{33} & \Delta_{34} \\
\Delta_{41} & \Delta_{42} & \Delta_{43} & \Delta_{44}
\end{bmatrix}
\begin{bmatrix}
E_x \\
H_y \\
E_z \\
H_x
\end{bmatrix}$$

$$\Rightarrow \frac{\partial}{\partial z} \mathbf{I}' = -i\omega \Delta \mathbf{I}'.$$ \hspace{1cm} (S1.9)

Herein \(\mathbf{I}'\) is the 4 × 1 generalized field vector and \(\Delta\) is a 4 × 4 differential propagation matrix, whose elements are functions of the elements of the optical matrix \(A\).
\[ \Delta_{11} = \rho_{12} + (\rho_{32} + \eta) (\rho_{13} \rho_{33} - \varepsilon_{31} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{23} (\rho_{33} \rho_{33} - \varepsilon_{33} \rho_{33}) / (\varepsilon_{33} \rho_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{22} = \mu_{22} + (\rho_{32} + \eta) (\mu_{23} \rho_{33} - (\rho_{32} + \eta) \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{23} (\rho_{33} + \eta) \mu_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{13} = \rho_{22} + (\rho_{32} + \eta) (\rho_{32} - \eta) \rho_{33} - \varepsilon_{32} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{14} = - \mu_{32} - (\rho_{32} + \eta) (\mu_{32} \mu_{33} - \varepsilon_{32} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{23} = \rho_{32} + \varepsilon_{33} (\mu_{32} \rho_{33} - \rho_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{33} = \rho_{32} + \varepsilon_{33} (\mu_{32} \rho_{33} - \rho_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{34} = \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{41} = \rho_{21} - (\rho_{21} + \eta) (\rho_{21} \rho_{33} - \varepsilon_{21} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{23} (\rho_{33} \rho_{33} - \varepsilon_{33} \rho_{33}) / (\varepsilon_{33} \rho_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{42} = \rho_{22} + (\rho_{32} + \eta) (\rho_{22} - \eta) \rho_{33} - \varepsilon_{22} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{43} = \rho_{23} + (\rho_{32} - \eta) \rho_{33} - \varepsilon_{32} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{33} \mu_{33} \rho_{33} - \varepsilon_{33} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta_{44} = \rho_{21} + (\rho_{32} + \eta) (\rho_{32} \mu_{33} - \varepsilon_{32} \mu_{33}) / (\varepsilon_{33} \mu_{33} - \rho_{33} \rho_{33}) + \mu_{23} (\rho_{33} \rho_{33} - \varepsilon_{33} \rho_{33}) / (\varepsilon_{33} \rho_{33} - \rho_{33} \rho_{33}) \]

\[ \Delta = \begin{bmatrix} 0 & \mu_{22} - (\eta^2 / \varepsilon_{33}) & 0 & 0 \\ \varepsilon_{33} & 0 & 0 & 0 \\ 0 & 0 & \mu_{33} & 0 \\ 0 & 0 & \varepsilon_{33} - (\eta^2 / \mu_{33}) & 0 \end{bmatrix} \]

Fig. S1 | Schematic diagram of the reflection and transmission of a plane wave by a stratified system.

\[ \rho (x + h) = e^{i \omega h} \rho (x) \]

where \( \eta = \zeta / \omega \). Regarding certain anisotropic media with a known \( \Delta \), the generalized field vector is specified by Eq. (S1.10). Even though the expression of \( \Delta \) seems to be too complicated, it can always be reduced to a relatively simple form. For example, the differential propagation matrix for an orthorhombic crystal with its principal axes parallel to the \( x, y, z \)-axes, which is a typical anisotropic medium\(^2\), has the following form

\[ \Delta = \begin{bmatrix} 0 & \mu_{22} - (\eta^2 / \varepsilon_{33}) & 0 & 0 \\ \varepsilon_{33} & 0 & 0 & 0 \\ 0 & 0 & \mu_{33} & 0 \\ 0 & 0 & \varepsilon_{33} - (\eta^2 / \mu_{33}) & 0 \end{bmatrix} \]

In the general case, Eq. (S1.9) does not have an analytical solution because the optical matrix \( \Delta \) is an arbitrary function of \( z \). Usually, we can subdivide the anisotropic medium into parts with a sufficiently thin length of \( h \), whose optical matrix is independent of \( z \). This yields the integration of Eq. (S1.9) as

\[ \Gamma (z + h) = e^{-i \omega h} \Gamma (z) \]

in which the exponential term can be Taylor expanded. Eq. (S1.13) describes a linear relation between the generalized field vectors at two different positions along the \( z \)-axis, separated by a distance of \( h \). This equation has four particular plane-wave solutions of the form
\[ I'(z) = I'_k(0) e^{-i\omega q_k z}, \quad k = 1, 2, 3, 4 \] (S1.13)

wherein \( q_k \) equals the component of the propagation vector of the plane wave along the z-axis. \( q_k \) have four values, which are the roots of the quartic polynomial equation

\[ \det [\omega \Delta q E] = 0, \] (S1.14)

where \( E \) is the 4 \( \times \) 4 identity matrix.

By using Eq. (S1.12), we can obtain the field vector relation between two parallel positions along the z-axis, and the calculation involving a certain distance \( d \) can be realized by the accumulation of thin thickness \( h \), written as

\[ I'(z + d) = e^{i\omega h_m \Delta z + d h_{m}} e^{i\omega h_2 \Delta z + h_1} e^{i\omega h_1 \Delta z} I'(z), \quad d = \sum_{i=1}^{m} h_i; \] (S1.15)

where \( \Delta x+h \) denotes the differential propagation matrix of the medium at the position of \( z + h \). Eq. S1.15 can be used to calculate the field vector numerically, and then the reflection and transmission properties with increased accuracy of the division length.

Section 2: Self-built fitness function setting and corresponding values

The evaluation factors of the self-built fitness function are shown in the main text. Herein we give the detailed function and its values.

Regarding the factor of the absolute intensity and contrast, we combine them together, then obtain

\[ f_1 + f_2 = 1 - \left( \frac{I_{\text{max}}^2 + I_{\text{max}} I_{\text{min}}}{I_{\text{max}} + I_{\text{min}}} \right). \] (S2.1)

It means that the weight factors \( w_1 \) and \( w_2 \) mentioned in the main text are both 0.5.

Regarding the factor of the linearity, we have

\[ f_3 = 0.1 \times \left( 2 (1 - R_{L_1}^2) + \frac{SSE_{L_1}}{2} + 2 (1 - R_{L_2}^2) + \frac{SSE_{L_2}}{2} \right) / (I_{\text{max}} - I_{\text{min}}), \] (S2.2)

where \( R_{L_1}^2 \) and \( SSE_{L_1} \) denote the R-squared value and sum of squares due to error of the part \( L_1 \) shown in Fig. 4 in the main text, and \( R_{L_2}^2 \) and \( SSE_{L_2} \) denote those of the part \( L_2 \). The scale factor of 0.1 and the weight factors 2 and 0.5 contained in the numerator are set to adjust \( f_3 \) to a value comparable to \( f_1 \) and \( f_2 \). In addition, the denominator is used to normalize the factor.

Regarding the factor of the symmetry, we have

\[ f_4 = \left| \max \{ L_1, L_2 \} - \frac{\lambda}{2} \right|. \] (S2.3)

Actually, the values of the weight factors are taken based on the probability distribution of each evaluation factor. As shown in Fig. S2, the settings defined in Eqs. (S2.1–S2.3) help to make each evaluation factor has a feasible weight in the overall fitness value. The absolute intensity, contrast \( f_1 \) and linearity \( f_2 \) are our major concerns, which are in the same order of magnitude. It is easy to adjust the factors in terms of different design goals. For example, the asymmetry condition expressed in Eq. (S2.3) can be readily changed to the symmetry condition by changing the component of \( \lambda/2 \) to \( \lambda/4 \).

![Fig. S2 | Histogram of the distribution of each evaluation factor for Ge/17 nm/Ag up-case setting.](220018-S4)
Section 3: Material library

Here we give a detailed list of the materials used in the inverse design. The simple substances, normal materials, and whole materials are listed in Table S1, wherein the gold color represents the simple substances, the orange color represents the normal materials, and the blue color represents whole materials. Although the table only lists the

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Table S1 | Detailed list of materials

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complex refractive index at 850 nm, we have established the database for a wide range of wavelengths, covering the commonly used wavelengths.

References


S27. Vos MFJ, Macco B, Thissen NFW, Bol AA, Kessels WM. Atomic layer deposition of molybdenum oxide from (NBu)2(NMe2)2Mo and O2 plasma. J Vac Sci Technol A 34, 01A103 (2016).


