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Active tuning of anisotropic phonon polaritons in natural van der Waals heterostructures by negative permittivity substrates and its application

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Section 1: Generation, reorientation and annihilation of in-plane hyperbolic polaritons in a slab embedded between two semi-infinite media

In this section, we derive the conditions under which the fundamental mode generates, reorientates and annihilates in a vdW slab surrounded between two semi-infinite media compared with the configuration embedded in air. The dielectric function of the substrate is negative while that of the superstrate is positive.

RB 1. In this case, $\varepsilon_x > 0$, $\varepsilon_y < 0$, $\varepsilon_z > 0$. Similar to the derivation shown in the main text, we set $\varphi = 0$ and therefore, $\rho = \mathrm{i}\sqrt{\varepsilon_z/\varepsilon_y}$. Since $\varepsilon_y < 0$ in RB 1, then $\mathrm{i}\sqrt{\varepsilon_z/\varepsilon_y} = -\sqrt{\varepsilon_z/\left|\varepsilon_y\right|}$ and Eq. (3) can be simplified as follow:

$$\tan\left(-\frac{kd}{\sqrt{\varepsilon_z/\left|\varepsilon_y\right|}}\right) = \frac{-\sqrt{\frac{\varepsilon_z}{\left|\varepsilon_y\right|}}\frac{(\varepsilon_1+\varepsilon_3)}{\varepsilon_z}}{1-\frac{\varepsilon_1\varepsilon_3}{\left|\varepsilon_y\right|\varepsilon_z}} , \tag{S1}$$

here $\frac{kd}{\sqrt{\varepsilon_z/\left|\varepsilon_y\right|}} > 0$, but also $\frac{kd}{\sqrt{\varepsilon_z/\left|\varepsilon_y\right|}} < \frac{\pi}{2}$ due to the model $l = 0$ is considered in this section. The left-hand side of Eq. (S1) is negative. Therefore, for Eq. (S1) to have a solution, the right-hand side must be also negative. Note that $\varepsilon_1 > 0$ and $\varepsilon_3 < 0$, namely, the denominator of the fraction in the right-hand side of Eq. (S1) is positive. Thus, for Eq. (S1) to have a solution, the numerator in the right-hand side of Eq. (S1) must be negative. Hence, we get the condition of propagation of polaritons along y axis:

$$\varepsilon_1+\varepsilon_3 > 0 . \tag{S2}$$

Analogously, let us study the reorientation of PhPs, namely, propagation direction of PhPs rotates from the y axis to x axis. In this case, we set $\phi = \frac{\pi}{2}$ and therefore, $\rho = \mathrm{i}\sqrt{\varepsilon_z/\varepsilon_x}$. Since $\varepsilon_x > 0$ in RB 2, $\sqrt{\varepsilon_z/\varepsilon_x}$ is positive and pure real. For the convenience of derivation, we set $\xi = \sqrt{\varepsilon_z/\varepsilon_x}$ (with ξ also positive and pure real). Thus Eq. (3) can be simplified as follow:

$$\tan\left(-\mathrm{i}\frac{kd}{\xi}\right) = \frac{\mathrm{i}\xi\frac{(\varepsilon_1+\varepsilon_3)}{\varepsilon_z}}{1+\frac{\varepsilon_1\varepsilon_3}{\varepsilon_z\varepsilon_x}} . \tag{S3}$$

Taking into account that tan is odd function and $\tan(\mathrm{i}\eta) = \mathrm{i}\tanh(\eta)$, Eq. (S3) can be rewritten as:

$$\tanh\left(\frac{kd}{\xi}\right) = \frac{-\xi\frac{(\varepsilon_1+\varepsilon_3)}{\varepsilon_z}}{1+\frac{\varepsilon_1\varepsilon_3}{\varepsilon_z\varepsilon_x}} . \tag{S4}$$

Note that the left-hand side of Eq. (S4) is positive, for Eq. (S4) have a solution, the right-hand side must be also positive, namely the sign of the denominator and numerator must be same. There are two cases, one is that if $\varepsilon_x\varepsilon_z+\varepsilon_1\varepsilon_3 < 0$, the condition where the polaritons can propagate along the x axis reads:

$$\varepsilon_1+\varepsilon_3 > 0 . \tag{S5}$$

The other is that if $\varepsilon_x\varepsilon_z+\varepsilon_1\varepsilon_3 > 0$ (the superstrate is low-permittivity media, such as air), the condition becomes

$$\varepsilon_1+\varepsilon_3 < 0 . \tag{S6}$$

Our analysis above shows that the HPhPs can propagate along the y axis in the range in which $\varepsilon_1+\varepsilon_3 > 0$, while propagate along the x axis, i.e., reorientation in the range $\varepsilon_1+\varepsilon_3 > 0$ or $\varepsilon_1+\varepsilon_3 < 0$ with respective assumptions. For the other case, i.e., $\varepsilon_1+\varepsilon_3 < 0$ and $\varepsilon_x\varepsilon_z+\varepsilon_1\varepsilon_3 < 0$, the fundamental mode annihilates, as listed in Table S1.

Table S1 | The state of fundamental mode of PhPs in RB 1.

RB 1: $\varepsilon_x > 0, \varepsilon_y < 0, \varepsilon_z > 0$			
State of fundamental mode (l= 0)	Propagation direction of polariton (l=0)	$\varepsilon_1, \varepsilon_3$	Assumption ($\varepsilon_1 >, \varepsilon_3 < 0$)
	y	$\varepsilon_1+\varepsilon_3>0$	None
Reorientation	*x*		$\varepsilon_x\varepsilon_z+\varepsilon_1\varepsilon_3<0$
		$\varepsilon_1+\varepsilon_3<0$	$\varepsilon_x\varepsilon_z+\varepsilon_1\varepsilon_3>0$
Annihilation	None		$\varepsilon_x\varepsilon_z+\varepsilon_1\varepsilon_3<0$

RB 3. In this case, $\varepsilon_x > 0$, $\varepsilon_y > 0$, $\varepsilon_z < 0$. The isofrequency contour of PhPs in this spectral band is elliptical or closed. And we know that when the α-MoO_3 slab is embedded by air, the fundamental mode is suppressed. However, the slab is placed on the substate with negative dielectric function, it is possible to excite the fundamental mode. Since $\varepsilon_z < 0$ in RB 3, then $\rho = -\sqrt{|\varepsilon_z|/\left(\varepsilon_x\cos^2\varphi+\varepsilon_y\sin^2\varphi\right)}$ is real and pure negative, so that Eq. (3) can be simplified,

$$\left(\frac{kd}{\rho}\right)=\frac{\dfrac{\rho\left(\varepsilon_1+\varepsilon_3\right)}{\varepsilon_z}}{1+\dfrac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x cos^2\alpha+\varepsilon_y sin^2\alpha\right)\varepsilon_z}}\ . \tag{S7}$$

Note that the left-hand side of Eq. (S7) is negative, for Eq. (S7) have a solution, the right-hand side must be also negative, namely the sign of the denominator and numerator must be different. Note that the sign of $\frac{\rho}{\varepsilon_z}$ is positive, so the sign of $\frac{\varepsilon_1+\varepsilon_3}{1+\frac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}}$ must be negative. If $\varepsilon_1+\varepsilon_3>0$ and $1+\frac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}<0$ or $\varepsilon_1+\varepsilon_3<0$ and $1+\frac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}>0$, the fundamental mode ($l = 0$) is generated. For other cases, the fundamental mode is still suppressed, as listed in Table S2.

Table S2 | The state of fundamental mode of PhPs in RB 3.

RB 3: $\varepsilon_x > 0, \varepsilon_y > 0, \varepsilon_z < 0$		
State of fundamental mode(l= 0)	$\varepsilon_1, \varepsilon_3$	Assumption ($\varepsilon_1 >, \varepsilon_3 < 0$)
	$\varepsilon_1+\varepsilon_3>0$	$1+\frac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}>0$
	$\varepsilon_1+\varepsilon_3<0$	$1+\frac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}<0$
Generation	$\varepsilon_1+\varepsilon_3<0$	$1+\frac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}>0$
	$\varepsilon_1+\varepsilon_3>0$	$1+\frac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}<0$

For other spectral regions, the conditions are derived by a similar treatment mentioned above. And the results are shown in Table S3 and S4.

Table S3 | The state of fundamental mode of PhPs in transition region from RB 1 to RB 2

Transition region from RB 1 to RB 2: $\varepsilon_x < 0$, $\varepsilon_y < 0$, $\varepsilon_z > 0$		
State of fundamental mode (l = 0)	ε_1, ε_3	Assumption (ε_1 >0, ε_3 <0)
Annihilation	$\varepsilon_1 + \varepsilon_3 > 0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}<0$
	$\varepsilon_1 + \varepsilon_3 < 0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}>0$
	$\varepsilon_1 + \varepsilon_3 > 0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}>0$
	$\varepsilon_1 + \varepsilon_3 < 0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\left(\varepsilon_x\cos^2\alpha+\varepsilon_y\sin^2\alpha\right)\varepsilon_z}<0$

Table S4 | The state of fundamental mode of PhPs in transition region from RB 2 to RB 3

Transition region from RB2 to RB 3: $\varepsilon_x < 0, \varepsilon_y > 0, \varepsilon_z < 0$			
State of fundamental mode (l= 0)	Propagation direction of polariton(l=0)	$\varepsilon_1, \varepsilon_3$	assumption ($\varepsilon_1 >, \varepsilon_3 < 0$)
Annihilation		$\varepsilon_1+\varepsilon_3<0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_x\varepsilon_z}>0$ and $1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_y\varepsilon_z}<0$
		$\varepsilon_1+\varepsilon_3>0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_x\varepsilon_z}<0$ and $1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_y\varepsilon_z}>0$
	x	$\varepsilon_1+\varepsilon_3<0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_x\varepsilon_z}<0$
		$\varepsilon_1+\varepsilon_3>0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_x\varepsilon_z}>0$
Reorientation	*y*	$\varepsilon_1+\varepsilon_3<0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_y\varepsilon_z}>0$
		$\varepsilon_1+\varepsilon_3>0$	$1+\dfrac{\varepsilon_1\varepsilon_3}{\varepsilon_y\varepsilon_z}<0$

Section 2: The dielectric function of SiC

The dielectric function of SiC can be described by the Lorentz model[S1,S2]:

$$\varepsilon\left(\omega\right)=\varepsilon_{\infty}\left(\frac{\omega^2-\omega_{\mathrm{LO}}^2-\mathrm{i}\gamma\omega}{\omega^2-\omega_{\mathrm{TO}}^2-\mathrm{i}\gamma\omega}\right)\ , \tag{S8}$$

where ε_∞ = 6.7 is the high-frequency dielectric constant, ω_{LO} = 1.825×10^{14} rad/s is the longitudinal optical (LO) phonon frequency, ω_{TO} = 1.494×10^{14} rad/s is transverse optical (TO) phonon frequency, and γ = 8.996×10^{11} rad/s is the damping model.

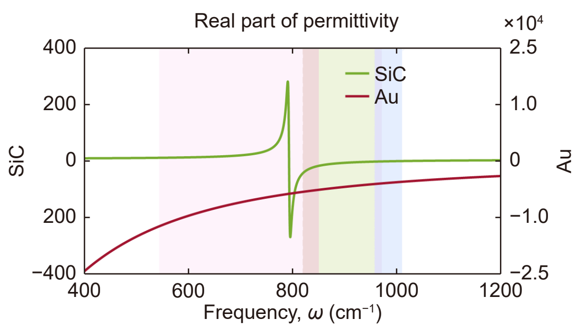

Fig. S1 | Real part of permittivity of substrates: SiC (left) and Au (right).

Section 3: The dielectric function of Au

The dielectric function of Au can be described by the Drude-Lorentz model[S3]:

$$\varepsilon\left(\omega\right)=\varepsilon_{\mathrm{D}}\left(\omega\right)+\varepsilon_{\mathrm{L}}\left(\omega\right)\ . \tag{S9}$$

The Drude term is given by

$$\varepsilon_D(\omega) = \varepsilon_\infty - \frac{\gamma\sigma}{\omega(\omega + i\gamma)} , \tag{S10}$$

where ε_∞ = 0.83409 is the high-frequency dielectric constant, σ = 3134.5 eV denotes the real DC conductivity. γ = 0.02334 eV represents the relaxation rate.

The Lorentz term is described by four pairs of poles

$$\varepsilon_L(\omega) = \sum_{k=1}^{4} \left(\frac{i\sigma_k}{\omega - \Omega_k} + \frac{i\sigma_k^*}{\omega + \Omega_k^*} \right) , \tag{S11}$$

where σ_k and Ω_k are the generalized conductivity and resonant frequency of the kth Lorentz pole, respectively. The parameters are listed in Table S5.

Table S5 | The parameters for Lorentz poles of gold.

*k*th	σ_x	Ω_x
1	−0.01743+i0.3059	2.6905−i0.16645
2	1.0349+i1.2919	2.8772−i0.44473
3	1.2274+i2.5605	3.7911−i0.81981
4	9.8+i37.614	4.8532−i13.891

Section 4: The generation and reorientation of PhPs in α-MoO_3 /Au heterostructure

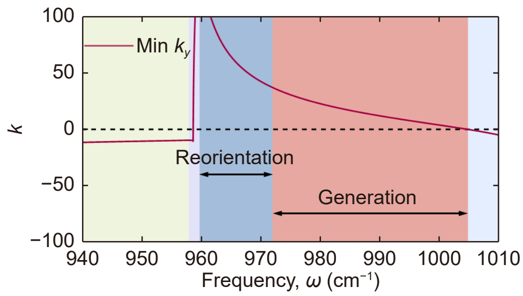

Fig. S2 | The minimum of k_y calculated by Eq.10. The blue and red shaded regions represent the reorientation and generation of fundamental mode of PhPs in α-MoO_3 /Au heterostructure, respectively.

Section 5: The derivation of the Transfer Matrix Method

The Transfer Matrix Method for general anisotropic materials is adopted to obtain the reflection matrix in our calculation. Note that there are two angles in our calculation, azimuth angle Φ and polarizing angle ψ. The former, azimuth angle Φ, denotes the angle between the plane of incidence and x-z plane as shown in Fig. S1. When Φ is not equal to zero, the plane of incidence is tilled off the x axis by an angle Φ. The latter, polarizing angle ψ, indicates the angle between the direction of polarization of the electric field and the plane of incidence. Consequently, $\psi = 0$ and $\frac{\pi}{2}$ corresponds to the transverse magnetic wave and transverse electric wave, respectively.

We consider the general case, the permittivity of material can be written in the form with reference to the xyz coordinate system:

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} . \tag{S12}$$

When the slab is rotated θ around the z axis, the permittivity tensor in the xyz coordinate system can be expressed as

$$\varepsilon = \boldsymbol{T}_z^{-1} \varepsilon \boldsymbol{T}_z , \tag{S13}$$

where T_z is the coordinate rotational transformation matrix and is the permittivity tensor before rotation. The matrix $\boldsymbol{T}_z$ is given as

$$\boldsymbol{T}_z = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{S14}$$

The electromagnetic fields in the incident medium are written as

$$\boldsymbol{E} = \boldsymbol{S}(z)\exp\left(\mathrm{j}\omega t - \mathrm{j}k_x x - \mathrm{j}k_y y\right) , \tag{S15}$$

and

$$\boldsymbol{H} = -\mathrm{j}\left(\varepsilon_0/\mu_0\right)^{1/2}\boldsymbol{U}(z)\exp\left(\mathrm{j}\omega t - \mathrm{j}k_x x - \mathrm{j}k_y y\right) , \tag{S16}$$

where $\boldsymbol{S} = (S_x, S_y, S_z)$ and $\boldsymbol{U} = (U_x, U_y, U_z)$.

Substituting Eqs. (S12), (S15) and (S16) into the Maxwell equations and setting $q_x = k_x / k_0$ and $q_y = k_y / k_0$, $z' = z * k_0$ we obtain the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}z'}\begin{pmatrix} S_x \\ S_y \\ U_x \\ U_y \end{pmatrix} = \boldsymbol{A}\begin{pmatrix} S_x \\ S_y \\ U_x \\ U_y \end{pmatrix} , \tag{S17}$$

where $\boldsymbol{A}$ is the coefficient matrix, which is the form

$$\boldsymbol{A} = \begin{bmatrix} \mathrm{i}\varepsilon_{zz}{}^{-1}\varepsilon_{zx}q_x & \mathrm{i}\varepsilon_{zz}{}^{-1}\varepsilon_{zy}q_x & -\varepsilon_{zz}{}^{-1}q_x q_y & -1+\varepsilon_{zz}{}^{-1}q_x^2 \\ \mathrm{i}\varepsilon_{zz}{}^{-1}\varepsilon_{zx}q_y & \mathrm{i}\varepsilon_{zz}{}^{-1}\varepsilon_{zy}q_y & 1-\varepsilon_{zz}{}^{-1}q_y^2 & \varepsilon_{zz}{}^{-1}q_x q_y \\ \varepsilon_{yz}\varepsilon_{zz}{}^{-1}\varepsilon_{zx} - \varepsilon_{yx} - q_x q_y & \varepsilon_{yz}\varepsilon_{zz}{}^{-1}\varepsilon_{zy} - \varepsilon_{yy} + q_x^2 & \mathrm{i}\varepsilon_{yz}\varepsilon_{zz}{}^{-1}q_y & \mathrm{i}\varepsilon_{yz}\varepsilon_{zz}{}^{-1}q_x \\ \varepsilon_{xx} - \varepsilon_{xz}\varepsilon_{zz}{}^{-1}\varepsilon_{zx} - q_y^2 & \varepsilon_{xy} - \varepsilon_{xz}\varepsilon_{zz}{}^{-1}\varepsilon_{zy} + q_x q_y & -\mathrm{i}\varepsilon_{xz}\varepsilon_{zz}{}^{-1}q_y & \mathrm{i}\varepsilon_{xz}\varepsilon_{zz}{}^{-1}q_x \end{bmatrix} . \tag{S18}$$

The differential equations in Eq. 6 describe the relation of tangential electromagnetic fields inside the anisotropic medium.

Assuming $\boldsymbol{U} = \begin{pmatrix} S_x & S_y & U_x & U_y \end{pmatrix}^{\mathrm{T}}$, we have $\boldsymbol{AU} = \boldsymbol{QU}$. By solving the equation, i.e. $|\boldsymbol{A} - \boldsymbol{QI}| = 0$, we obtain four eigenvalues Q_m, m=1,2,3,4 of matrix $\boldsymbol{A}$ and responding eigenvectors

$$\boldsymbol{\omega}_m = \begin{pmatrix} w_{1,m} \\ w_{2,m} \\ w_{3,m} \\ w_{4,m} \end{pmatrix}, m = 1,2,3,4 . \tag{S19}$$

Therefore, the electromagnetic field inside the medium can be described by the eigenvalues and eigenvectors

$$\begin{pmatrix} S_x(z) \\ S_y(z) \\ U_x(z) \\ U_y(z) \end{pmatrix} = c_1\begin{bmatrix} w_{1,1} \\ w_{2,1} \\ w_{3,1} \\ w_{4,1} \end{bmatrix}\exp\left(k_0 Q_1 z\right) + c_2\begin{bmatrix} w_{1,2} \\ w_{2,2} \\ w_{3,2} \\ w_{4,2} \end{bmatrix}\exp\left(k_0 Q_2 z\right)$$

$$+ c_3\begin{bmatrix} w_{1,3} \\ w_{2,3} \\ w_{3,3} \\ w_{4,3} \end{bmatrix}\exp\left(k_0 Q_3 z\right) + c_4\begin{bmatrix} w_{1,4} \\ w_{2,4} \\ w_{3,4} \\ w_{4,4} \end{bmatrix}\exp\left(k_0 Q_4 z\right) , \tag{S20}$$

where c_{m} is the coefficient and can be determined by matching the boundary conditions. Furthermore, we can divide Q into two categories by value of their real part: positive and negative. The real part of Q is positive, indicating the wave propagates forward, and vice versa, backward. Without loss of generality, we assume Re (Q_3) and Re(Q_4) are both positive while Re(Q_1) and Re(Q_2) are negative. With these assumptions, we can derive the electromagnetic fields for the infinite medium, which are written as

$$\begin{pmatrix} S_x(z) \\ S_y(z) \\ U_x(z) \\ U_y(z) \end{pmatrix} = c_1\begin{bmatrix} w_{1,1} \\ w_{2,1} \\ w_{3,1} \\ w_{4,1} \end{bmatrix}\exp\left(k_0 Q_1 z\right) + c_2\begin{bmatrix} w_{1,2} \\ w_{2,2} \\ w_{3,2} \\ w_{4,2} \end{bmatrix}\exp\left(k_0 Q_2 z\right) . \tag{S21}$$

The reflection and transition coefficients can be solved by applying the continuum of the tangential electric and magnetic fields components at the top and bottom interface of the medium, respectively. The boundary conditions depend on the polarization of incident light. In this paper, only linearly polarized light is considered: s- and p-polarized, so that we derive the boundary conditions of the transverse electric wave (s wave) and transverse magnetic wave (p wave), respectively.

If the incident wave is the transverse electric wave, the tangential electromagnetic fields at the top air-medium interface (inside air) can be written as

$$\begin{pmatrix} S_x^+(0) \\ S_y^+(0) \\ U_x^+(0) \\ U_y^+(0) \end{pmatrix} = \begin{pmatrix} \frac{k_z}{k_0}\cos\phi \\ \frac{k_z}{k_0}\sin\phi \\ -\mathrm{j}\sin\phi \\ \mathrm{j}\cos\phi \end{pmatrix} + \begin{pmatrix} \cos\phi & -\sin\phi & 0 & 0 \\ \sin\phi & \cos\phi & 0 & 0 \\ 0 & 0 & \cos\phi & -\sin\phi \\ 0 & 0 & \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} -\frac{k_z}{k_0} & 0 \\ 0 & 1 \\ 0 & j\frac{k_z}{k_0} \\ j & 0 \end{pmatrix} \begin{pmatrix} r_{sp} \\ r_{ss} \end{pmatrix} . \tag{S22}$$

From Eq. S21, we obtain the electromagnetic fields at the bottom air-medium interface (inside the medium), given by

$$\begin{pmatrix} S_x^-(0) \\ S_y^-(0) \\ U_x^-(0) \\ U_y^-(0) \end{pmatrix} = c_1^+ \begin{bmatrix} w_{1,1} \\ w_{2,1} \\ w_{3,1} \\ w_{4,1} \end{bmatrix} + c_2^+ \begin{bmatrix} w_{1,2} \\ w_{2,2} \\ w_{3,2} \\ w_{4,2} \end{bmatrix} + c_1^- \begin{bmatrix} w_{1,3} \\ w_{2,3} \\ w_{3,3} \\ w_{4,3} \end{bmatrix} \exp\left(-k_0 Q_3 t\right) + c_2^- \begin{bmatrix} w_{1,4} \\ w_{2,4} \\ w_{3,4} \\ w_{4,4} \end{bmatrix} \exp\left(-k_0 Q_4 t\right) . \tag{S23}$$

At the top medium-substrate interface (inside the medium), the tangential electric and magnetic fields components are written as

$$\begin{pmatrix} S_x^+(d) \\ S_y^+(d) \\ U_x^+(d) \\ U_y^+(d) \end{pmatrix} = c_1^+ \begin{bmatrix} w_{1,1} \\ w_{2,1} \\ w_{3,1} \\ w_{4,1} \end{bmatrix} \exp\left(k_0 Q_1 t\right) + c_2^+ \begin{bmatrix} w_{1,2} \\ w_{2,2} \\ w_{3,2} \\ w_{4,2} \end{bmatrix} \exp\left(k_0 Q_2 t\right) + c_1^- \begin{bmatrix} w_{1,3} \\ w_{2,3} \\ w_{3,3} \\ w_{4,3} \end{bmatrix} + c_2^- \begin{bmatrix} w_{1,4} \\ w_{2,4} \\ w_{3,4} \\ w_{4,4} \end{bmatrix} . \tag{S24}$$

For the transmission, the expression of tangential electromagnetic fields depends on the substrate. Here, we consider the general case, namely, the substrate medium is also made of anisotropic material. Hence, we use the Eq. (S9) to calculate the electromagnetic fields of the transmission medium, written as

$$\begin{pmatrix} S_x^-(d) \\ S_y^-(d) \\ U_x^-(d) \\ U_y^-(d) \end{pmatrix} = c_{2,1}^+ \begin{bmatrix} w_{1,1}^2 \\ w_{2,1}^2 \\ w_{2,1}^2 \\ w_{2,1}^2 \end{bmatrix} + c_{2,2}^+ \begin{bmatrix} w_{1,2}^2 \\ w_{2,2}^2 \\ w_{3,2}^2 \\ w_{3,2}^2 \end{bmatrix} . \tag{S25}$$

The continuum of the tangential electric and magnetic fields components at the top and bottom interface of the medium asks that:

$$\begin{pmatrix} S_x^+(0) \\ S_y^+(0) \\ U_x^+(0) \\ U_y^+(0) \end{pmatrix} = \begin{pmatrix} S_x^-(0) \\ S_y^-(0) \\ U_x^-(0) \\ U_y^-(0) \end{pmatrix} , \tag{S26}$$

and

$$\begin{pmatrix} S_x^+(d) \\ S_y^+(d) \\ U_x^+(d) \\ U_y^+(d) \end{pmatrix} = \begin{pmatrix} S_x^-(d) \\ S_y^-(d) \\ U_x^-(d) \\ U_y^-(d) \end{pmatrix} . \tag{S27}$$

The reflection coefficient, r_{sp} and r_{ss} can be solved by combining Eqs. (S22–S27).

For another case, namely, the incident wave is transverse magnetic wave, the tangential electric and magnetic field components are given by

$$\begin{pmatrix} S_x^+(0) \\ S_y^+(0) \\ U_x^+(0) \\ U_y^+(0) \end{pmatrix} = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ -\mathrm{j}\dfrac{k_z}{k_0}\cos\phi \\ -\mathrm{j}\dfrac{k_z}{k_0}\sin\phi \end{pmatrix} + \begin{pmatrix} \cos\phi & -\sin\phi & 0 & 0 \\ \sin\phi & \cos\phi & 0 & 0 \\ 0 & 0 & \cos\phi & -\sin\phi \\ 0 & 0 & \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} -\dfrac{k_z}{k_0} & 0 \\ 0 & 1 \\ 0 & \mathrm{j}\dfrac{k_z}{k_0} \\ \mathrm{j} & 0 \end{pmatrix} \begin{pmatrix} r_{pp} \\ r_{ps} \end{pmatrix}. \tag{S28}$$

Similarly, the reflection coefficient, r_{pp} and r_{ps} can be solved by combining Eqs. (S23–S28).

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