Supplemental Document

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Fast computation of scattering by isolated defects in periodic dielectric media: supplement

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Fast Computation of Scattering by Isolated Defects in Periodic Dielectric Media: supplemental document

1. AB-INITIO CALCULATION OF NEAR FIELDS

The internal electric fields discussed in the main text are calculated using the Finite Difference Time Domain (FDTD) method implemented in the package MEEP [1]. Bloch periodicity is employed in the plane of the structure, the x-y plane, and perfectly matched layers (PMLs) at the top and the bottom of the structure. Excitation was created with a current sheet $\hat{j}e^{i\boldsymbol{\kappa}\cdot\boldsymbol{r}_\perp - i\omega t}p(t)$, where $\boldsymbol{\kappa}$ is the projection of the wavevectors onto the plane of the structure. The source is multiplied by a finite Gaussian time-dependent pulse, $p(t)$, with center frequency corresponding to 200 nm and bandwidth to 50 nm. The calculations were run until the magnitude of the field in the upper-half-space vanished below 10^{-4}. The resulting time-dependent fields were analyzed using harmonic inversion [1] and the field components for the frequency corresponding to the wavelength of 200 nm were extracted.

To account for the strong dispersion of the materials in the frequency regime of interest, MEEP couples the Maxwell equations to polarization source terms that are themselves driven by the electric fields [1]. The total polarization is modeled as a sum of simpler polarization fields each evolving as a driven harmonic oscillator. In frequency domain, this corresponds exactly to a linear dielectric function with the Lorentzian dispersion,

$$\varepsilon(\omega) = \left(1 + \frac{i\sigma_D}{2\pi\omega}\right)\left[\varepsilon_\infty + \sum_{n=1}^{N}\frac{\omega_n^2\sigma_n}{\omega_n^2 - \omega^2 - i\omega\gamma_n}\right] \tag{S1}$$

The parameters of this oscillator model are fit to the optical constants data [2] over the limited range of wavelengths from 195 nm to 300 nm. I performed model selection by varying N from 1 to 5 to obtain the best fit results. The results for Mo and SiO_2 are shown in figure S1. Mo data corresponds to $N = 5$ and SiO_2 data to $N = 1$. I show the parameters for the metal lines, Mo, in Table S1.

As discussed in the text, the ground truth scattering matrix of the defect is generated using the exact overlap integral between the time-reversed background field $\boldsymbol{E}^{(0)}$ and the induced polarization inside the defect volume. Due to the periodic boundary conditions in the lateral dimensions, these dimensions must be large enough to suppress the effect of neighboring defects placed periodically. Letting this dimension be L, we write the scattering matrix as,

$$\Delta S_L(\boldsymbol{k}_\alpha, \hat{e}_\alpha; \boldsymbol{k}'_\beta, \hat{e}_\beta) = \frac{-ik^2}{2E_0\epsilon_0 k_z}\sum_i \int_{V^d} \mathrm{d}^3\boldsymbol{r}\boldsymbol{E}_L^{(0)}(\boldsymbol{r}; -\boldsymbol{\kappa}, \hat{e})\boldsymbol{P}_L^{(d)}(\boldsymbol{r}; \boldsymbol{\kappa}', \hat{e}')\text{..} \tag{S2}$$

The exact scattering matrix of the periodic array of defects is

$$\Delta S_{per}(\boldsymbol{k}_\alpha, \hat{e}_\alpha; \boldsymbol{k}'_\beta, \hat{e}_\beta) = \Delta S_L(\boldsymbol{k}_\alpha, \hat{e}_\alpha; \boldsymbol{k}'_\beta, \hat{e}_\beta)\sum_{\boldsymbol{R}} e^{i(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\cdot\boldsymbol{R}}, \tag{S3}$$

where $\boldsymbol{R}$ are the lattice vectors and the summation represents the structure factor in the form of delta functions located in the wave-vector space at the reciprocal lattice vectors. However, if the structure factor is ignored, then the scattering matrix of an *isolated defect* is obtained in the limit, $L \to \infty$, *i.e..*,

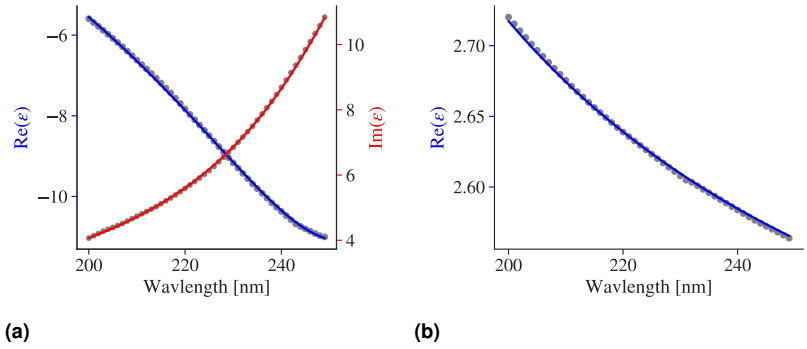
$$\Delta S_{iso}(\boldsymbol{k}_\alpha, \hat{e}_\alpha; \boldsymbol{k}'_\beta, \hat{e}_\beta) = \lim_{L\to\infty} \Delta S_L(\boldsymbol{k}_\alpha, \hat{e}_\alpha; \boldsymbol{k}'_\beta, \hat{e}_\beta) \tag{S4}$$

Note that due to the overlap integral in the definition of ΔS_L being restricted to lie inside the defect volume, the field solutions $\boldsymbol{E}_L$ must converge only inside the defect volume, placed farthest from the boundaries, and it must converge only in the integral sense and not necessarily point-wise. In structures with sufficiently high absorption, L need not be very large before

	$\omega_n/2\pi$	$\gamma_n/2\pi$	σ_n
0	0.001964	0.000198	27.496889
1	0.003658	0.000912	3.057252
2	0.006121	0.013024	1.531705
3	0.008171	0.059215	7.372552
4	0.010273	0.086407	0.690262

Table S1. Parameters of the Lorentz oscillator model Eq. (S1) for Mo. The fit results are shown in S1. The parameter $\varepsilon_\infty = 2.08$ and $\sigma_D = 0$.

convergence is achieved. Furthermore, the approach to this limit does not impact the ability to fit the parameters of the susceptibility tensor. It only leads to an overall scaling. In this work, I found that $L > 100nm$ suffices for the Mo/SiO_2 line space system at a wavelength of 200 nm. When the length scale for the scattered field inside the structure is governed by absorption, the wavelength plays only a secondary role in determining the dimensions of the domain through the dispersion relation $\epsilon(\omega)$. This is another direct benefit of using the formula Eq. (S2) to compute the scattering matrix in contrast to computing it by the difference of scattering matrices in the presence and absence of the defect. The latter require the domain size to be directly governed by the number of propagating modes allowed by the Bloch periodicity of the structure.



(a) **(b)**

Fig. S1. (a) Real and imaginary parts of the dielectric function of Mo. The gray dots are data from Palik while the solid lines are produced by the analytical model Eq. (S1) with $N = 5$. (b) Real part of the dielectric function of SiO2 with data from Palik (dots) and the Lorentzian model fit with $N = 1$.

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