Simulating Huygens' Surfaces

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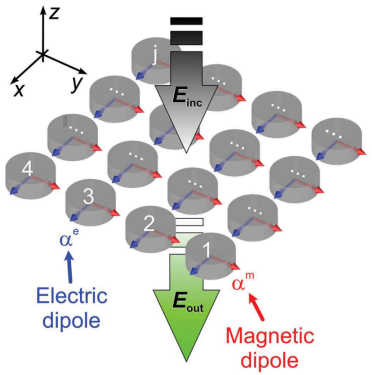


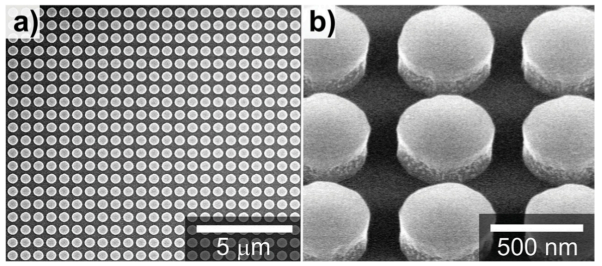


Figure 3. a) Top-view and b) side-view electron micrographs of a typical silicon-nanodisk sample with a disk radius of $r_d \approx 242$ nm, a disk height of $h = 220$ nm, and a lattice constant of $a \approx 666$ nm.

Figure 1: Huygens Metasurface

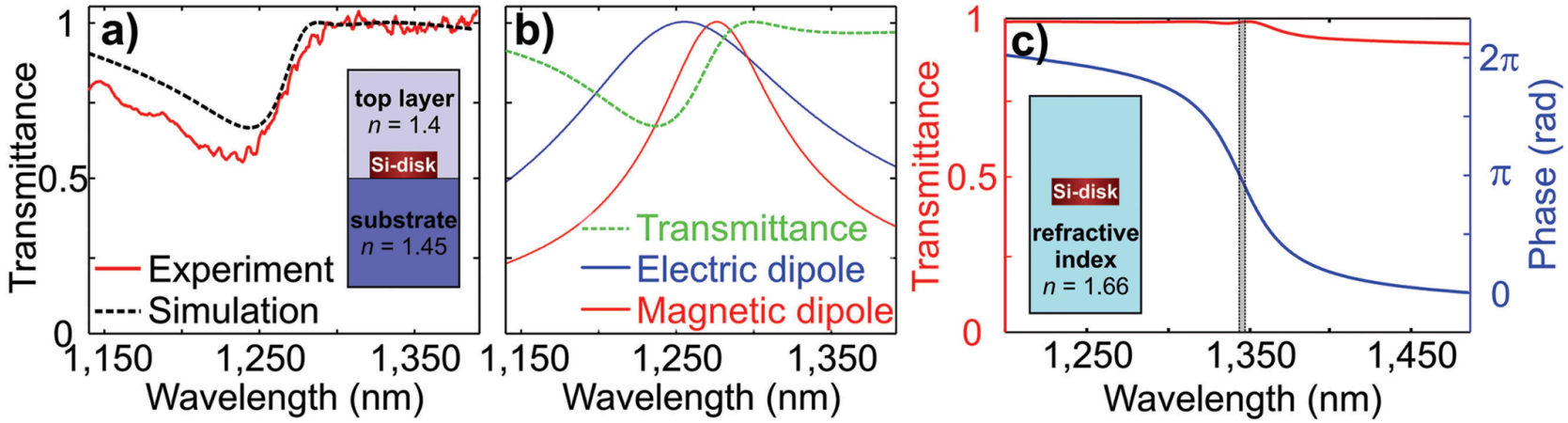


Figure 5. a) Experimental transmittance spectrum of the Huygens' metasurface [overlap case shown in Figure 4b)] embedded in spin-on glass ($n = 1.4$) after handle-wafer removal (red-solid line) and corresponding numerical calculation (black-dashed line). b) Transmittance intensity (green line) gained from the analytical model and its decomposition into electric (blue) and magnetic (red) dipole contributions. The parameters for the electric and

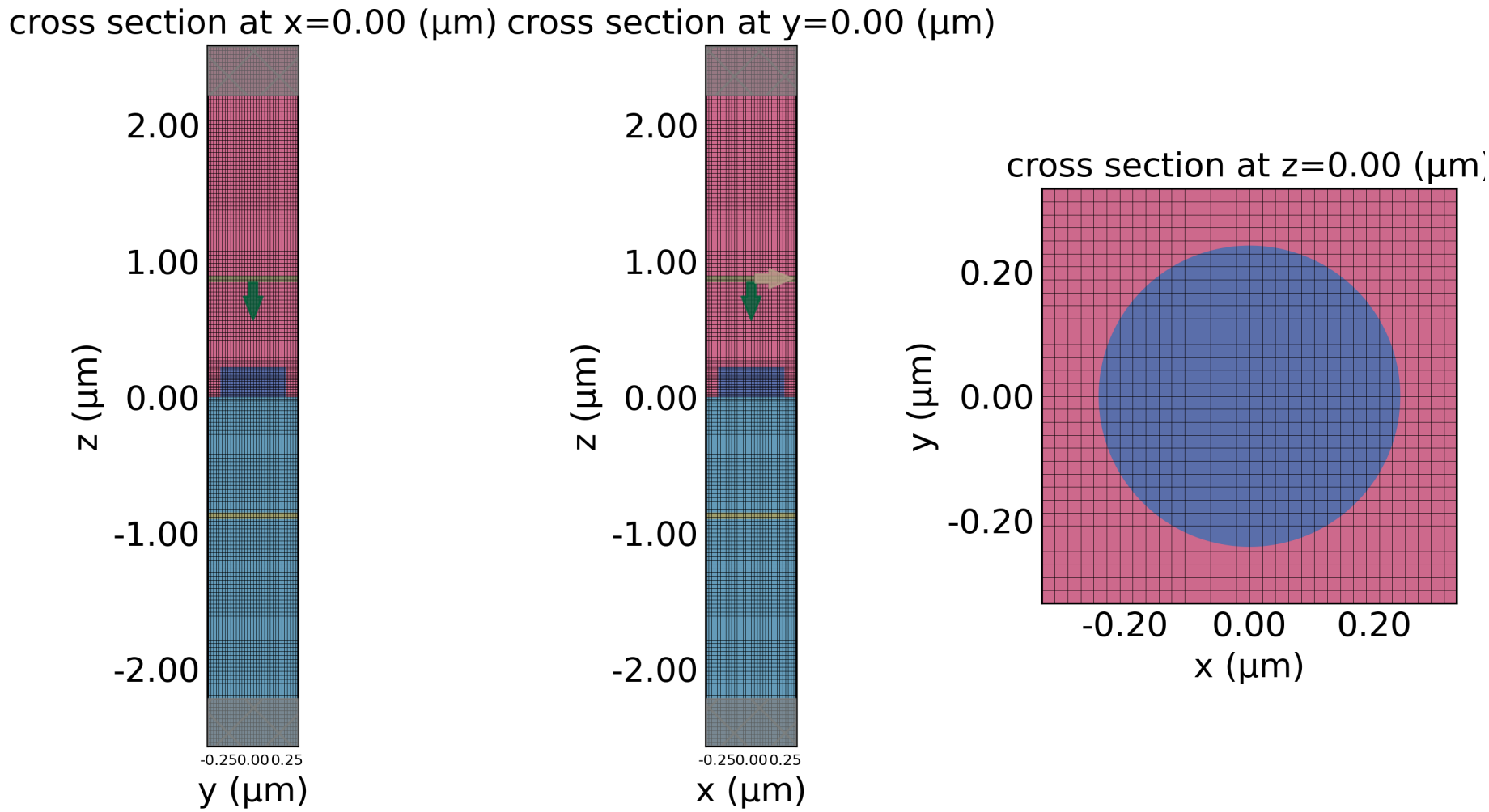
Simulation Overview

```python
# Import the necessary packages
import matplotlib.pyplot as plt
import numpy as np
import tidy3d as td
import tidy3d.web as web
import scienceplots

# Set logging level to ERROR to reduce output verbosity
td.config.logging_level = "ERROR"
```

For the transmittance and phase, two different background materials were used based in the paper, so two separate simulations were ran (with background medium as the only difference).

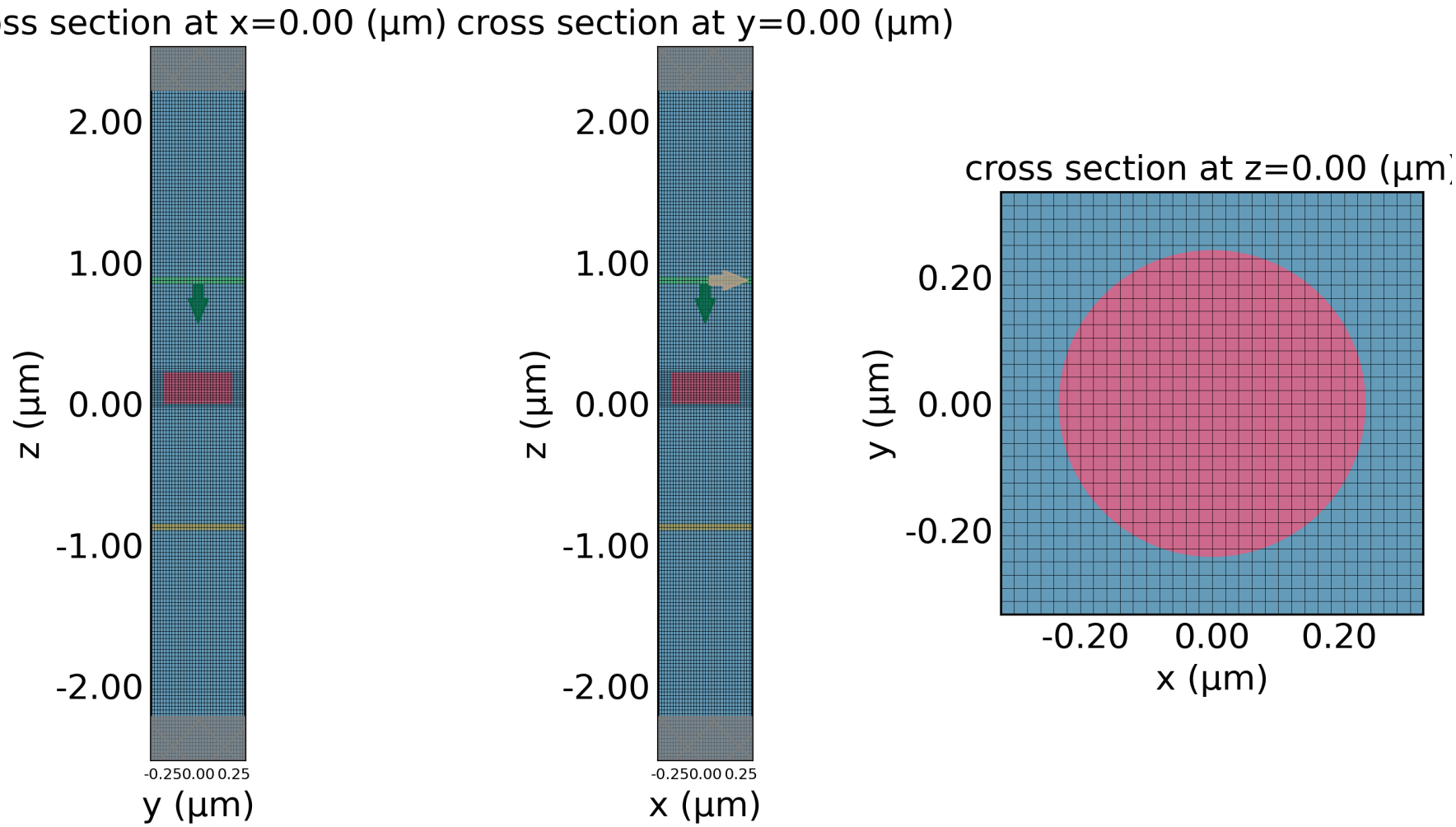
Note: Several other technical variables need to be changed. In tidy3D simulation, transmittance should be measured with `td.FluxMonitor` and phase should be measured with `td.FieldMonitor`. The `run_time` also needs to increase since the background medium has a higher refractive index in the second simulation than the first, so waves will travel more slowly.

Simulation 1



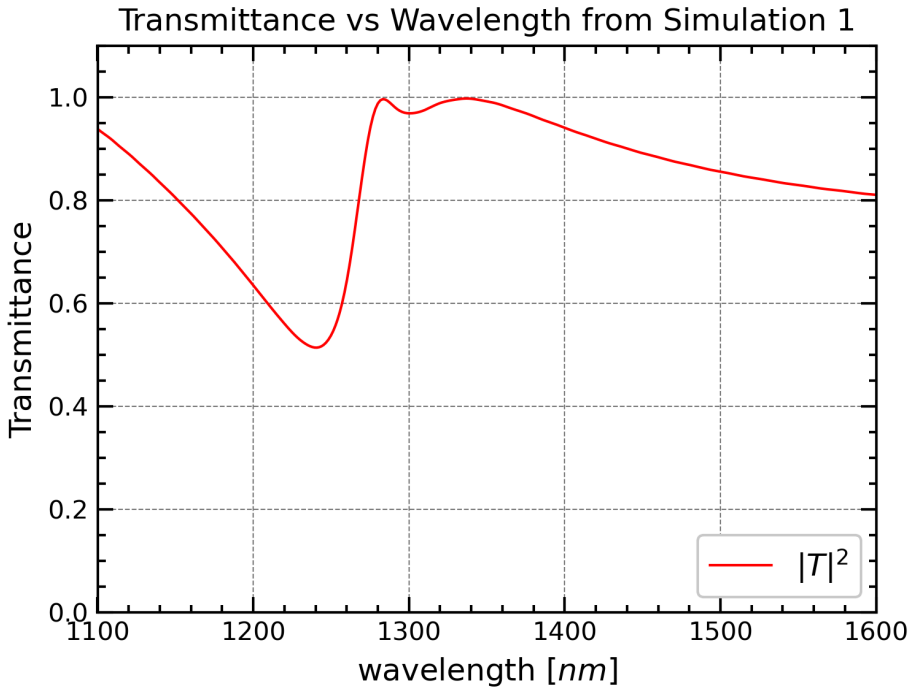
Top Layer n=1.4, Bottom Layer n=1.45

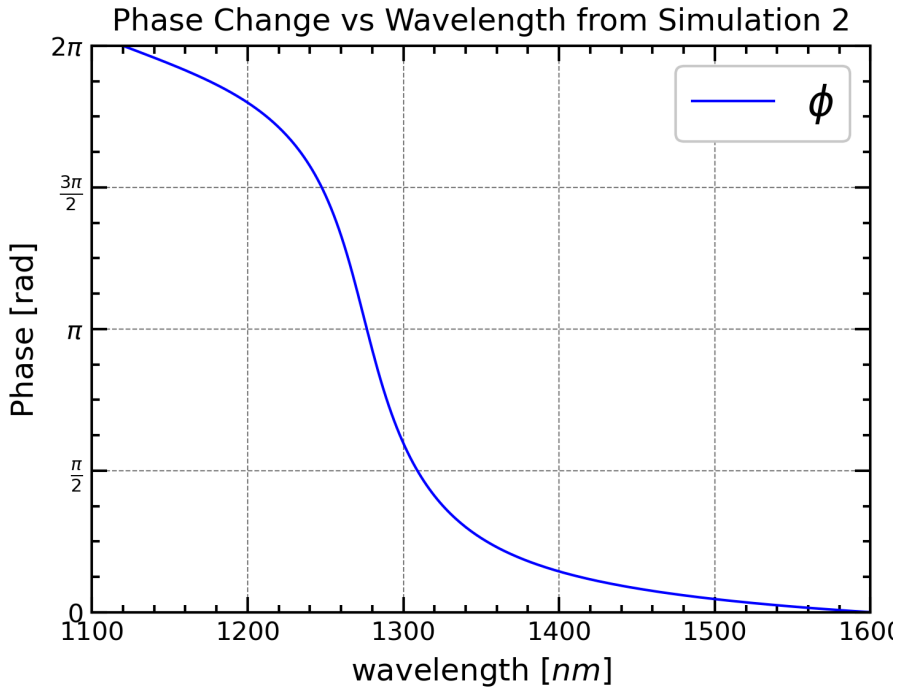
Simulation 2



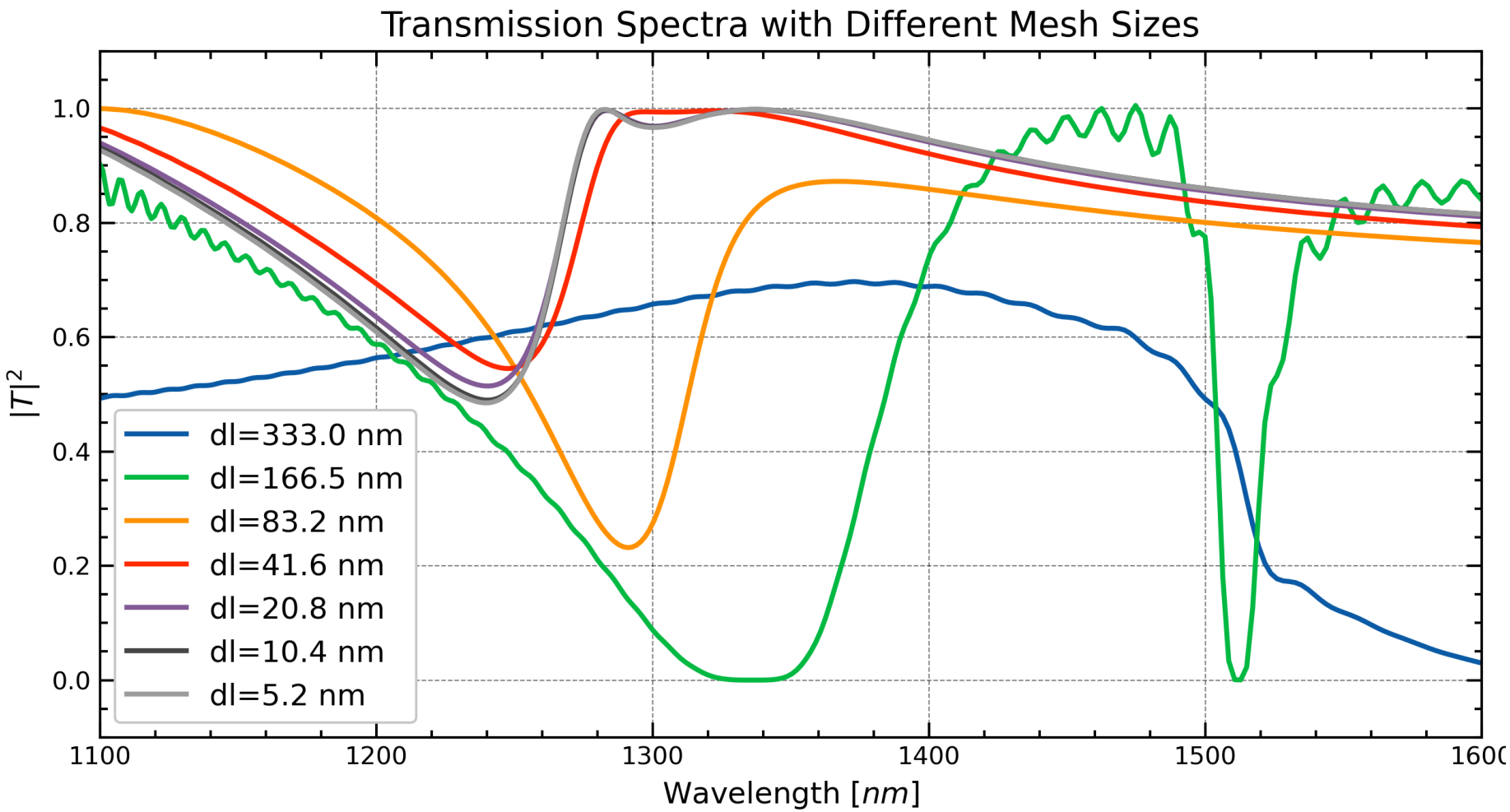
Background medium n=1.66

Simulation Results





Mesh Study Results



Convergence of Transmittance

Initialization

Here we follow the seven steps of initialization I wrote down in the tutorial:

0. Frequency Range Specification
1. Computational Domain Size
2. Grid Specifications (Discretization size)
3. Structures and Materials
4. Sources
5. Monitors
6. Run time
7. Boundary Condition Specification

o Frequency Range Specification

```python
# 0 Define a FreqRange object with desired wavelengths
fr = td.FreqRange.from_wvl_interval(wvl_min=1.1, wvl_max=1.6)
N = 301 # num_points
freq0 = fr.freq0
lda0 = td.C_0 / fr.freq0
```

1 Computational Domain Size

```
# 1 Computational Domain Size
h = 0.220  # Height of cylinder
spc = 2
Lz = spc + h + h + spc

Px = Py = P = 0.666 # periodicity
sim_size = [Px, Py, Lz]
```

2 Grid Resolution

Grid resolution is uniform grid in the horizontal direction with a yee cell length of $\frac{P}{32}$ where P is the periodicity. In the vertical direction, `AutoGrid` means it's non-uniform and adjusted based on the wavelength of the particular medium. Here, `min_steps_per_wvl=32` means we are taking a minimum of 32 steps based on the wavelength, which will be shorter in the medium with a higher index of refraction.

```
# 2 Grid Resolution
dl = P / 32
horizontal_grid = td.UniformGrid(dl=dl)
vertical_grid = td.AutoGrid(min_steps_per_wvl=32)
grid_spec=td.GridSpec(
    grid_x=horizontal_grid,
    grid_y=horizontal_grid,
    grid_z=vertical_grid,
)
```

3 Structures and Materials

Structures and Materials for the meta-atom

```
r = 0.242  # radius of the cylinder
n_Si = 3.5
Si = td.Medium(permittivity=n_Si**2, name='Si')
cylinder = td.Structure(
    geometry=td.Cylinder(center=[0, 0, h / 2], radius=r, length=h, axis=2), medium=Si
)
```

Background Medium for Figure 5(a) ($n_1 = 1.4, n_2 = 1.45$)

```
# Background medium for the first simulation
n_glass = 1.4
n_SiO2 = 1.45
glass = td.Medium(permittivity=n_glass**2, name='glass')
SiO2 = td.Medium(permittivity=n_SiO2**2, name='oxide')

substrate = td.Structure(
    geometry=td.Box(
        center=(0,0,-Lz/2),
        size=(td.inf,td.inf,2 * (spc+h))
    ),
    medium=SiO2,
    name='substrate'
)

```

4 The Source

The source is a simple Plane wave that traverses in the -z axis, placed $\frac{\lambda_0}{2}$ distance above the metaatom in the computational domain. Polarization is along the x-axis, that's what `pol_angle=0` means.

```
source = td.PlaneWave(
    source_time=fr.to_gaussian_pulse(),
    size=(td.inf, td.inf, 0),
    center=(0, 0, Lz/2 - spc + 0.5 * lda0),
    direction="-",
    pol_angle=0
)
```

5 Monitors

Monitor for Transmittance

```
flux_monitor = td.FluxMonitor(
    center=(0, 0, -Lz/2 + spc - 0.5 * lda0),
    size=(td.inf, td.inf, 0),
    freqs=fr.freqs(N),
    name="flux_monitor"
)
```

Monitor for Phase

```
# We use FieldMonitor instead of DiffractionMonitor because
# DiffractionMonitor only gives you amplitudes of diffraction orders,
# losing phase detail if you care about continuous phase.
field_monitor = td.FieldMonitor(
    center=(0, 0, -Lz/2 + spc - 0.5 * lda0),
    size=(td.inf, td.inf, 0),
    fields=["Ex"],
    freqs=fr.freqs(N),
    name="field_monitor"
)
```

6 Run Time

```
bandwidth = fr.fmax - fr.fmin
run_time_short = 50 / bandwidth # run_time for the transmittance simulation
run_time_long = 200 / bandwidth # run_time for the phase simulation
```

7 Boundary Conditions

We apply PML in the +Z and -Z surfaces.

```
bc = td.BoundarySpec(
    x=td.Boundary.periodic(),
    y=td.Boundary.periodic(),
    z=td.Boundary.pml()
)
```

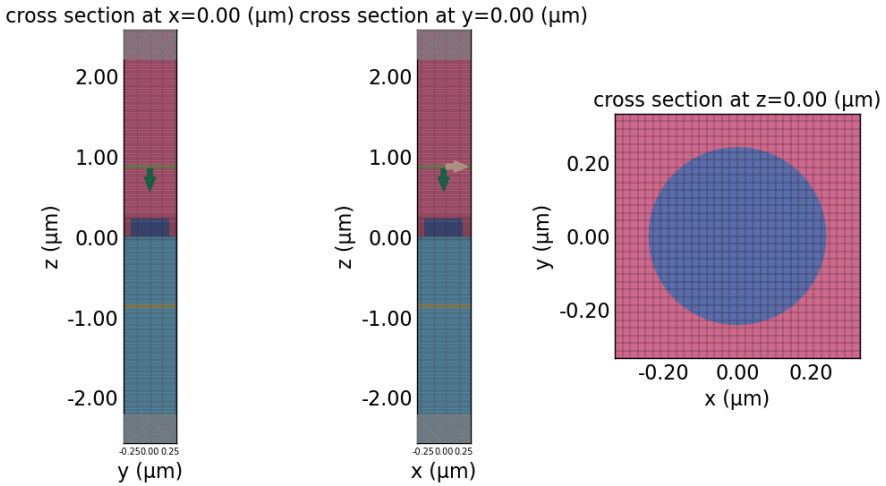
Helper Function for simulation

Since we have to run simulation two times, it is convenient to abstract out what are the differences to the two simulations and make defining simulations easier. Always follow the DRY Principle.

```
def simulation_helper(background, monitors, run_time):
    """
    Create normalization and actual tidy3d simulations, visualize geometry,
    and return both as a dictionary.

    Parameters
    ----------
    background : list of td.Structure
        Background structures (without the cylinder).
    monitors : list of td.Monitor
        Monitors for the normalization run.
    run_time : float
        Run time for the normalization simulation.

    Returns
    -------
    dict
        {"norm": Simulation without cylinder,
         "actual": Simulation with cylinder}

    Notes
```

Transmittance Simulation

```
sims = simulation_helper(
    background=[substrate, glass],
    monitors=[flux_monitor],
    run_time=run_time_short
)
```



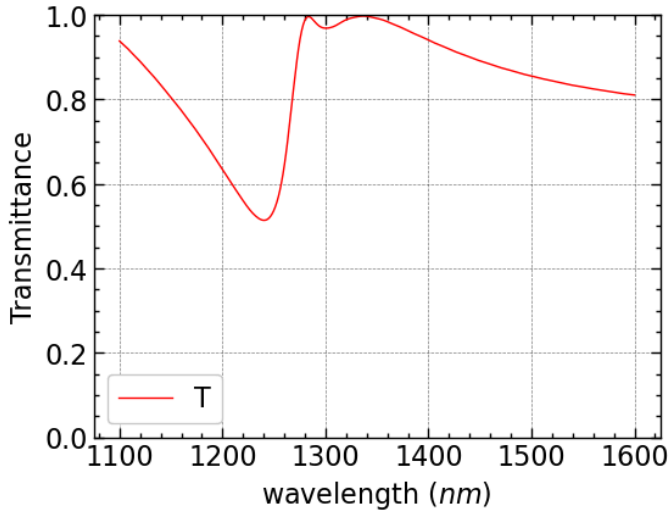

```
batch = web.Batch(simulations=sims, verbose=True)
batch_data = batch.run(path_dir="data/huygens5a")
```

```
02:20:56 EDT Started working on Batch containing 2 tasks.
02:20:57 EDT Maximum FlexCredit cost: 0.050 for the whole batch.
             Use 'Batch.real_cost()' to get the billed FlexCredit cost after the
             Batch has completed.
02:20:58 EDT Batch complete.
```

Transmittance Results

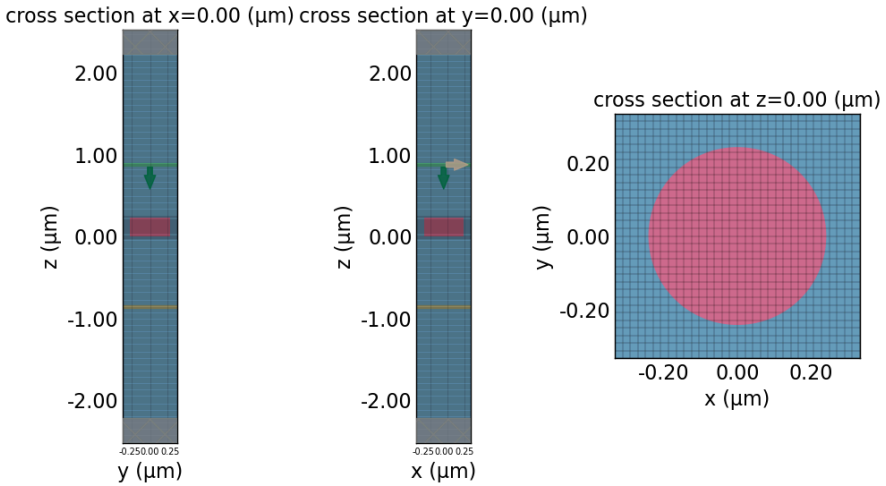
```python
# this uses scienceplots to make plots look better
plt.style.use(['science', 'notebook', 'grid'])
T = batch_data["actual"]["flux_monitor"].flux / batch_data["norm"]["flux_monitor"].flux
```

```python
# plot transmission, compare to paper results, look similar
fig, ax = plt.subplots(1, 1, figsize=(6, 4.5))
plt.plot(td.C_0 / fr.freqs(N) * 1000, np.abs(T)**2, "r", lw=1, label="T")
plt.xlabel(r"wavelength ($nm$)")
plt.ylabel("Transmittance")
plt.ylim(0, 1)
plt.legend()
plt.show()
```



Phase Simulation

```
sims = simulation_helper(
    background=[polymer],
    monitors=[field_monitor],
    run_time=run_time_long
)
```




```
batch = web.Batch(simulations=sims, verbose=True)
batch_data = batch.run(path_dir="data/huygens5c")
```

```
02:21:11 EDT Started working on Batch containing 2 tasks.
02:21:13 EDT Maximum FlexCredit cost: 0.050 for the whole batch.
             Use 'Batch.real_cost()' to get the billed FlexCredit cost after the
             Batch has completed.
02:21:14 EDT Batch complete.
```

Phase Results

```python
# Data Extraction
Ex_actual = batch_data["actual"]["field_monitor"].Ex
Ex_norm = batch_data["norm"]["field_monitor"].Ex
Ex = Ex_actual / Ex_norm
```

```python
# 1. Compute average over the xy-plane
Ex_avg = np.mean(Ex[:, :, 0, :], axis=(0,1))

# 2. Compute phase
phase_avg = np.angle(Ex_avg)

# 3. Unwrap phase to remove ±pi jumps
phase_avg_unwrapped = np.unwrap(phase_avg)

# 4. Make relative to first point (optional)
phase_rel = phase_avg_unwrapped - phase_avg_unwrapped[0]

phase_actual = np.unwrap(np.angle(np.mean(Ex_actual[:, :, 0, :], axis=(0,1))))
phase_norm = np.unwrap(np.angle(np.mean(Ex_norm[:, :, 0, :], axis=(0,1))))
```

```python
fig, ax = plt.subplots(1, 1, figsize=(6, 4.5))
plt.plot(td.C_0 / fr.freqs(N) * 1000, phase_rel, "r", lw=1, label="$\phi$")
plt.plot(td.C_0 / fr.freqs(N) * 1000, phase_actual, "b", lw=1, label="Actual $\phi$")
plt.plot(td.C_0 / fr.freqs(N) * 1000, phase_norm, "g", lw=1, label="Norm $\phi$")
plt.xlabel(r"wavelength ($nm$)")
plt.ylabel("Phase")
plt.legend()
```

Final Plotting

```
fig, axes = plt.subplots(1, 2, figsize=(12, 4))

# work on the first figure
ax = axes[0]
ax.tick_params(axis="both", labelsize=10)
ax.plot(td.C_0 / fr.freqs(N) * 1000, np.abs(T)**2, "r", lw=1, label="$|T|^2$")
ax.set_xlabel(r"wavelength [$nm$]", fontsize=12)
ax.set_ylabel("Transmittance", fontsize=12)
ax.set_title("Transmittance vs Wavelength from Simulation 1", fontsize=12)
ax.set_xlim(1100, 1600)
ax.set_ylim(0, 1.1)
ax.legend(loc="lower right", fontsize=12)

# work on the second figure
ax = axes[1]
ax.tick_params(axis="both", labelsize=10)
ax.plot(td.C_0 / fr.freqs(N) * 1000, phase_rel, "b", lw=1, label="$\phi$")
ax.set_xlabel(r"wavelength [$nm$]", fontsize=12)
ax.set_ylabel("Phase [rad]", fontsize=12)
ax.set_title("Phase Change vs Wavelength from Simulation 2", fontsize=12)
ax.set_xlim(1100, 1600)
ax.set_ylim(0, np.pi*2)
yticks = [0, np.pi/2, np.pi, 3*np.pi/2, 2*np.pi]
ytick_labels = [r"$0$", r"$\frac{\pi}{2}$", r"$\pi$",
                r"$\frac{3\pi}{2}$", r"$2\pi$"]
ax.set_yticks(yticks)
ax.set_yticklabels(ytick_labels)
```

Mesh Study

Here, we set out to study the effect of different yee cell length on the transmittance.

```
dls = [P/2, P/4, P/8, P/16, P/32, P/64, P/128] # mesh study list
sims = {}
```

```
# for each dl in dls
for i, dl in enumerate(dls):
    # 2 Grid Specifications
    horizontal_grid = td.UniformGrid(dl=dl)
    vertical_grid = td.AutoGrid(min_steps_per_wvl=32)
    grid_spec=td.GridSpec(
        grid_x=horizontal_grid,
        grid_y=horizontal_grid,
        grid_z=vertical_grid,
    )

    # 4 Sources
    source = td.PlaneWave(
        source_time=fr.to_gaussian_pulse(),
        size=(td.inf, td.inf, 0),
        center=(0, 0, Lz/2 - spc + 2 * dl),
        direction="-",
        pol_angle=0
    )

```

Mesh Study Results

```python
# Extract results
x = td.C_0 / fr.freqs(N) * 1000
Ts = []
for i in range(len(dls)):
    Ts.append(batch_data[f"actual{i}"]["flux"].flux / batch_data[f"norm{i}"]["flux"].flu
```

```python
# Plot results
plt.figure(figsize=(10, 5))
for i, T in enumerate(Ts):
    plt.plot(x, np.abs(T)**2, "-",lw=1, label=f"dl={dls[i] * 1000:.1f} nm")
plt.xlabel(r"Wavelength [$nm$]", fontsize=12)
plt.ylabel(r"$|T|^2$", fontsize=12)
plt.xlim(1100, 1600)
plt.ylim(-0.1, 1.1)
plt.legend(fontsize=12)
plt.tick_params(axis='both', labelsize=10) # change tick label size to 10
plt.title("Transmission Spectra with Different Mesh Sizes", fontsize=14)
plt.savefig("mesh_convergence.png", dpi=300)
plt.show()
```