Optical Polarization Response of Hybrid Gratings Made of Metals and Polymers Based on Bruggeman Theory

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Supporting Information

1. Simulation parameters

The simulation is composed of five primary components: the FDTD region, the simulation structure (rectangular grating), the source, the reflection monitor, and the transmission monitor. All parameters are defined and controlled through a script integrated within the model.

FDTD Simulation Region:

The FDTD simulation was performed in two dimensions, as the structure exhibits uniformity along the z-axis allowing for effective modeling on the xy plane. Furthermore, the simulation was designed with periodic boundary conditions in the Y-direction, reflecting the repeating nature of the structure along this axis. This approach captures the behavior of the periodic elements while minimizing computational costs.

There are two important factors for consideration of the simulation settings along the x-axis. One of them is the length of simulation region in x direction and the other one is the PML (perfectly matched layer).

We observed that an insufficient x-axis length caused inaccuracies in the simulation results by limiting complete light propagation. To address this, we performed convergence tests to determine the optimal simulation length, which was found to be 3.5 μm of free space, plus the structure's physical length.

The PML is set to the previously determined steep angle profile within the simulation settings. According to Lumerical FDTD's documentation, this profile is recommended when periodic boundary conditions are present. To evaluate the suitability of steep angle PML profile, we added a movie monitor to observe the distribution of total power. The steep angle PML profile ensures that no artificial reflections occur and that all light passing through the PML layer is absorbed efficiently.

Structure (Rectangular Grating):

The grating structure is positioned at the center of the simulation region, with its length along the x-axis set to 20 nm for all simulations. All other parameters are set according to the descriptions provided in the main text.

Source:

The source is positioned 125 nm away from the grating along the x-axis extending across the entire y-axis.

Monitors:

The reflection and transmission monitors are positioned 350 nm away from the start and end of the simulation region along the x-axis.

Material fitting and material settings:

As explained in the main text, refractive indices of materials made of different compositions of gold, silver, and PDMS are calculated. These refractive indices are added to the simulation using Lumerical python API. The tolerance is set to 10^{-6} and maximum number of coefficients is set to 10. The fitting of the refractive indices to the calculated data are carried out by the Lumerical FDTD between the wavelengths of 300 and 1500 nm. The stability of the results is tested by employing convergence tests.

Meshing:

Uniform meshing with 1 nm resolution is employed as the mesh setting.

2. Statistical analyses

The simulations produced polarization-dependent transmission and reflection spectra for each simulated material composition and structural parameters. To reveal the effect of these variables on the polarization ratio, we studied the peak values of the polarization ratios and the corresponding wavelengths for the transmitted and reflected light.

- Polarization ratio's peak wavelengths for all the material and structural parameter combinations: All polarization peak wavelengths are found; their averages and standard deviations are calculated for the reflected and transmitted light, separately.
- Polarization ratio's peak values for all the material and structural parameter combinations:
  Peak polarization ratios were determined; their averages and standard deviations are calculated for the reflected and transmitted light separately.
- Silver-Gold concentration effect on the peak polarization ratio wavelength:
  Considering all the structural parameters, we calculated the peak polarization ratios and corresponding wavelengths for each material combination. For each PDMS concentration, we grouped the peak polarization wavelength data in five groups belonging to five different combinations of silver-gold concentrations simulated (see Methodology section in the main text). Next, for each PDMS concentration, we determined the average of how much the peak polarization wavelengths change per 1% increase in gold concentration. Finally, considering all the PDMS concentrations, we calculated the average and standard deviation of the change in the peak polarization wavelength with respect to 1% increase in the gold concentration increase.

- PDMS concentration effect on the peak polarization ratio wavelength:

  For each PDMS concentration, we calculated the average of the peak polarization ratio wavelengths and calculated the average and standard deviations in the shift of this wavelength per 2% change in the PDMS concentration.

- Grating constant effect on the peak polarization ratio wavelength:
  Analyses of the effect of grating constant on the peak polarization ratio wavelength was carried also using a similar approach. For each grating constant, the average peak polarization ratio wavelengths were determined and the average shift of this wavelength and its standard deviation per 1 nm change in the grating were calculated.

3. Maxwell-Garnett approximation validation results

Alloy modeling was performed using Maxwell Garnett's approximations as outlined in the article. To validate our results, we referenced another study that investigates the refractive index of gold-silver alloys. We then applied the Maxwell-Garnett mixture calculations. Figure S1 illustrates the refractive index modeling of the original sample and compares it with the results obtained from ellipsometry.

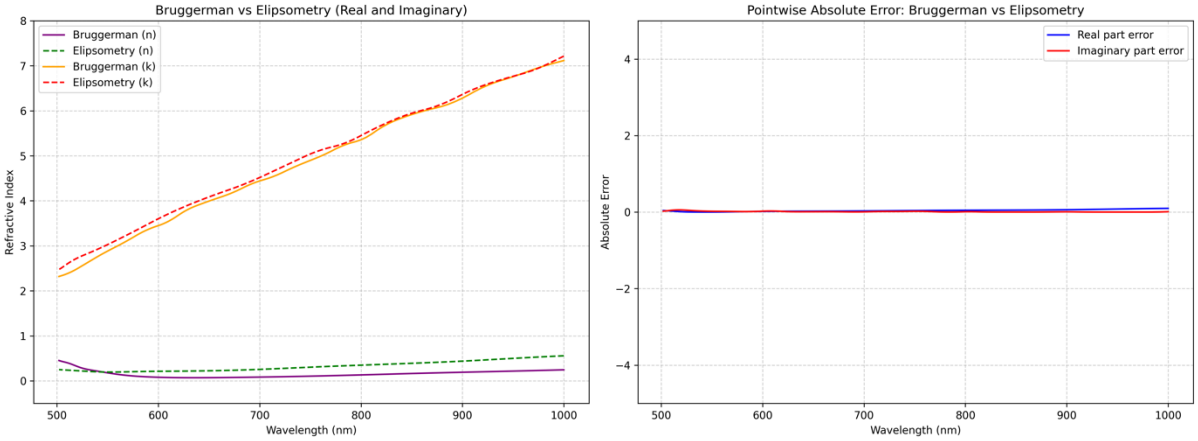

Figure S1. Comparison of the ellipsometry measurement of a 52% gold and 48% silver mix with Bruggeman theory. The left subfigure displays the direct refractive index comparison of the experimental measurement (Ellipsometry) and the effective medium approximation (Bruggeman), while the right subfigure illustrates the difference between them.

4. Raw simulation results

All simulation results for different structural parameters and different material compositions are presented below:

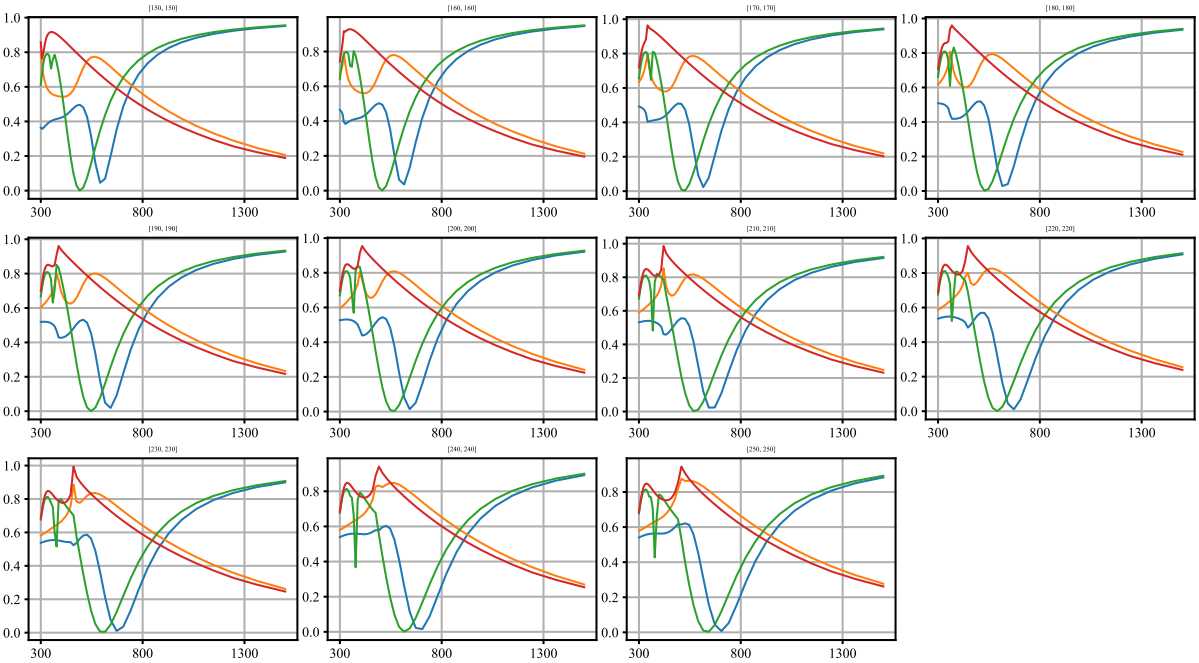

Figure S2. Transmission spectra of the gratings for parallel and perpendicularly polarized light. The subtitle of each subfigure represents the width (W), and the distance between gratings (G-W) (see Figure 1 in the main text), respectively. Red, orange, green, and blue lines indicate the transmission spectra of silver gratings (perpendicular polarization), gold gratings (perpendicular polarization), silver gratings (parallel polarization), and gold gratings (parallel polarization), respectively.

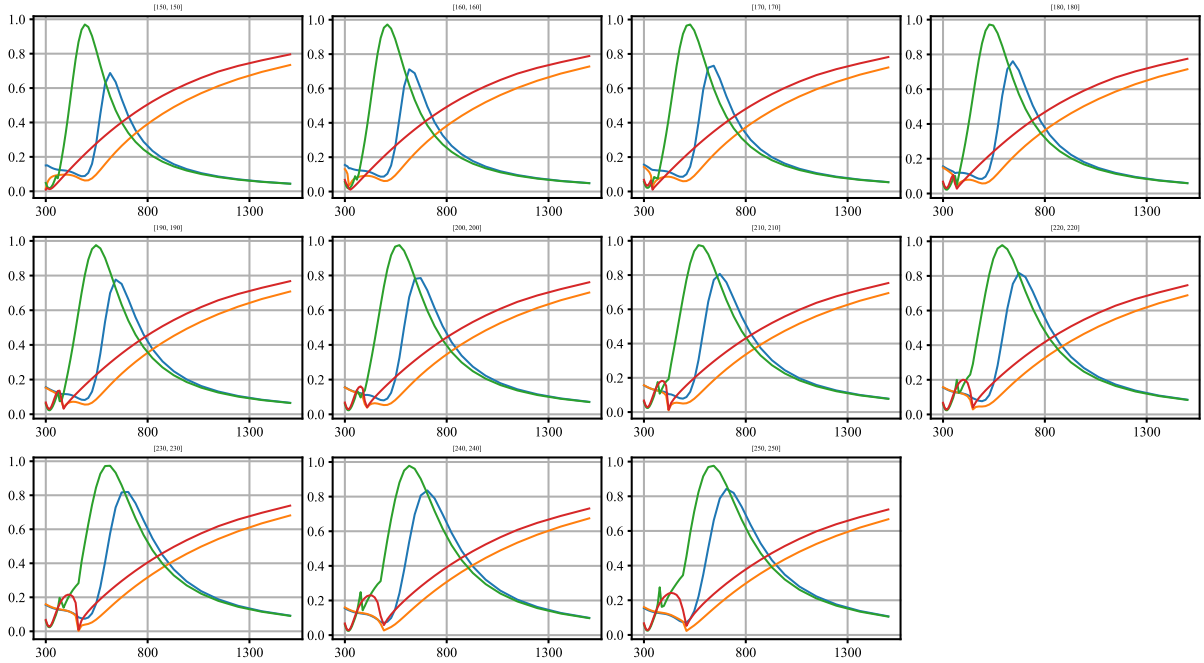

Figure S3. Reflection spectra of the gratings for parallel and perpendicularly polarized light. The subtitle of each subfigure represents the width (W), and the distance between gratings (G-W) (see Figure 1 in the main text), respectively. Red, orange, green, and blue lines indicate the reflection spectra of silver gratings (perpendicular polarization), gold gratings (perpendicular polarization), silver gratings (parallel polarization), and gold gratings (parallel polarization), respectively.

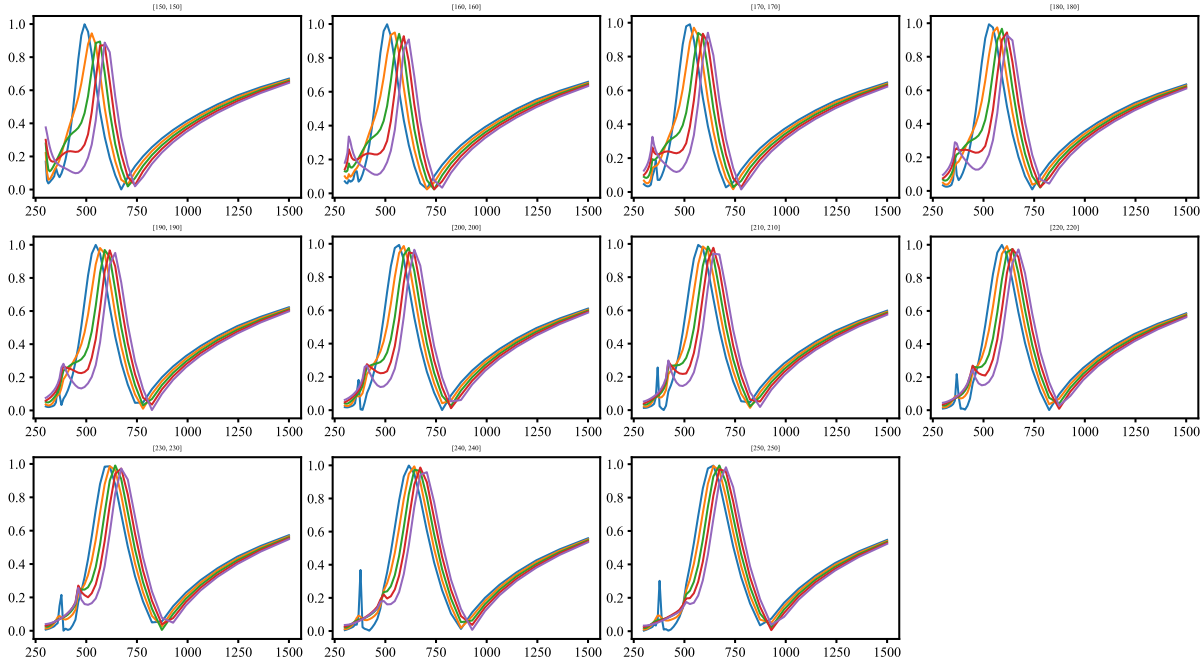

Figure S4. Polarization ratio of the transmitted light for the grating materials that contain 0% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

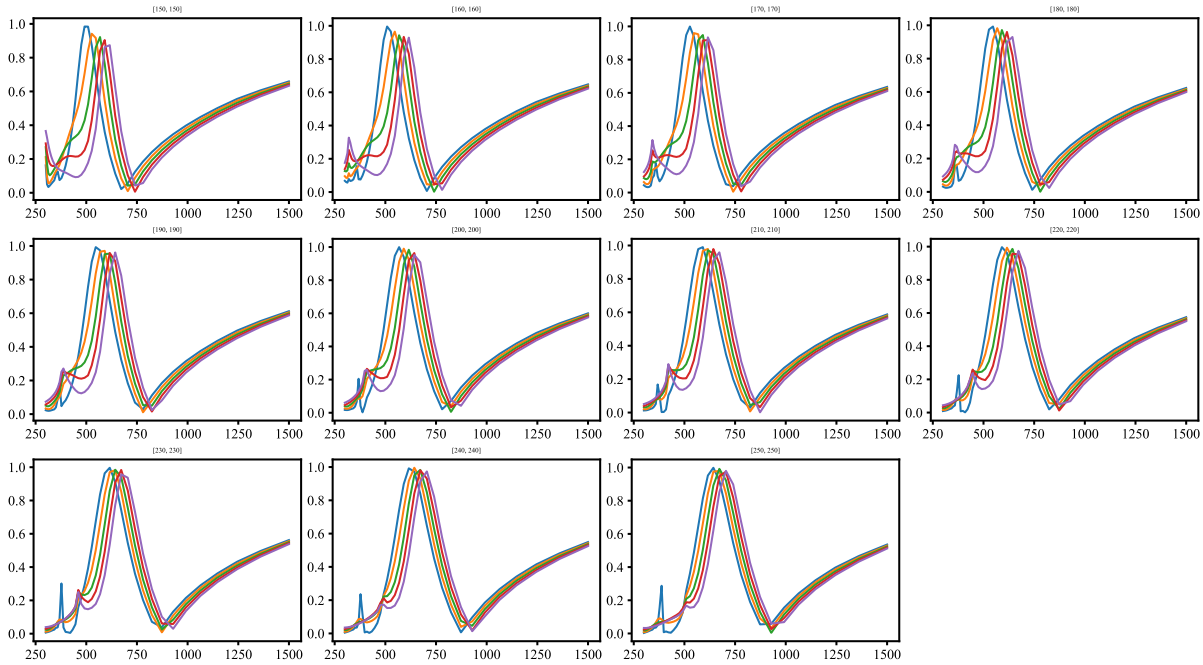

Figure S5. Polarization ratio of the transmitted light for the grating materials that contain 2% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

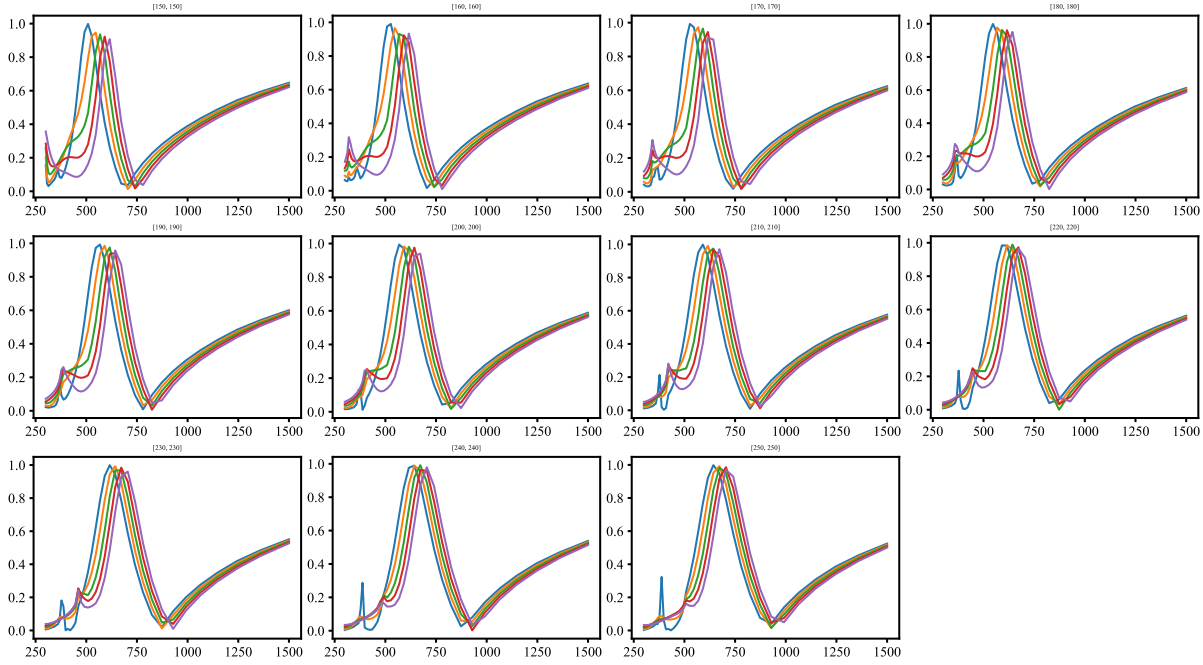

Figure S6. Polarization ratio of the transmitted light for the grating materials that contain 4% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

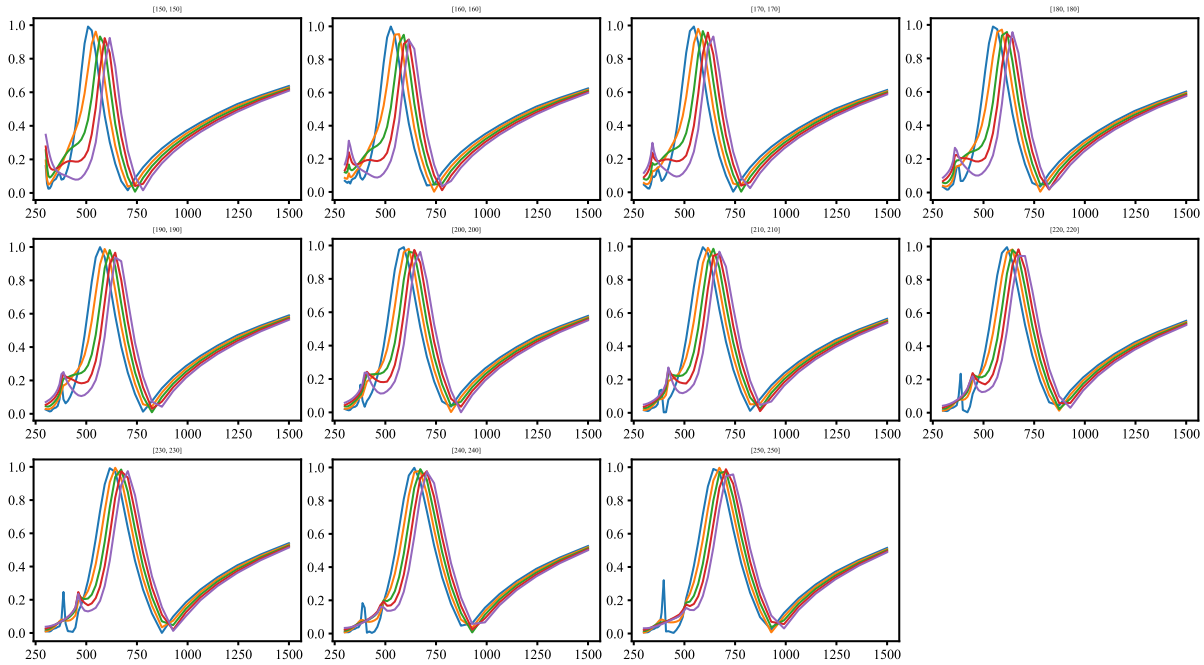

Figure S7. Polarization ratio of the transmitted light for the grating materials that contain 6% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

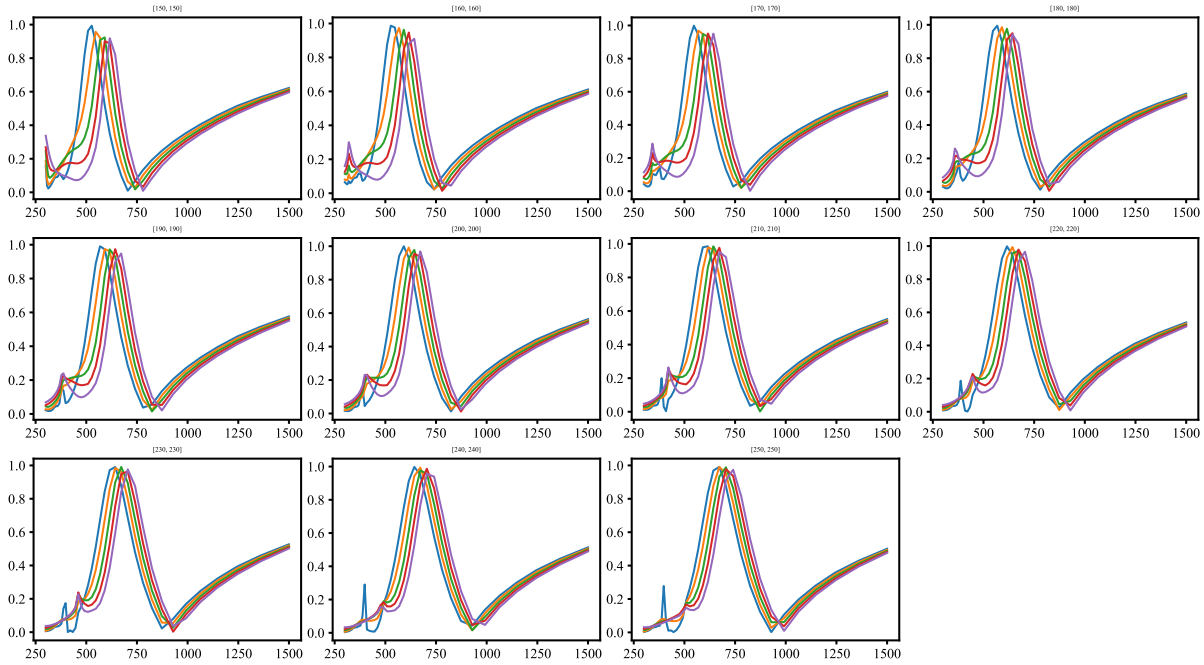

Figure S8. Polarization ratio of the transmitted light for the grating materials that contain 8% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

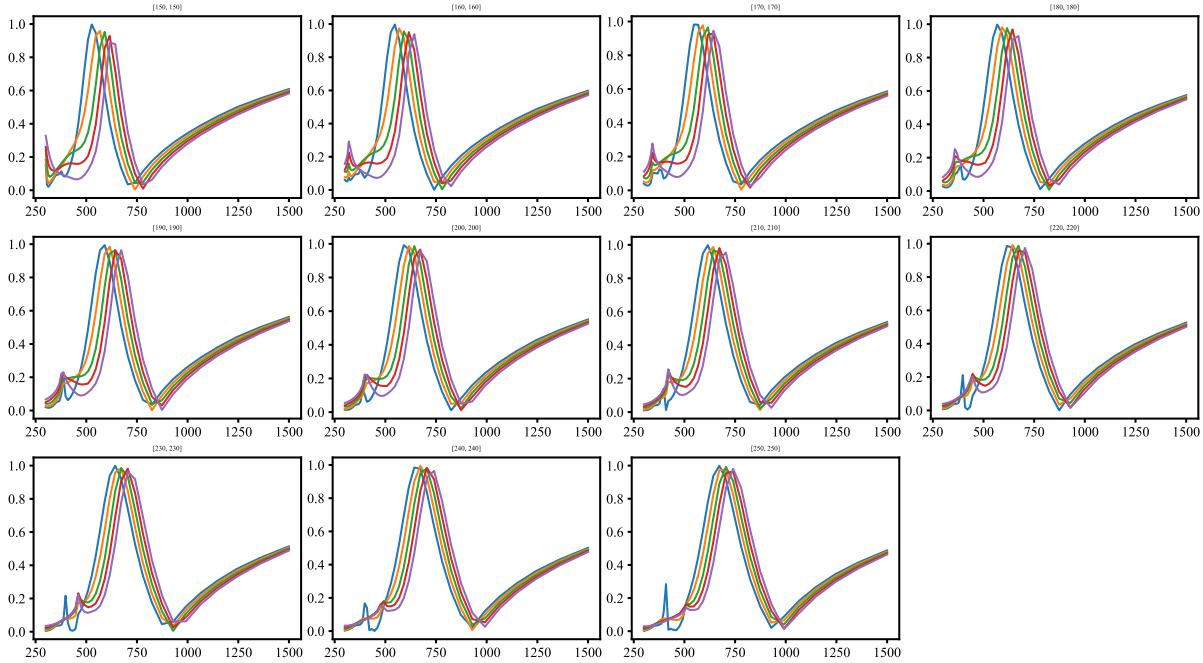

Figure S9. Polarization ratio of the transmitted light for the grating materials that contain 10% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

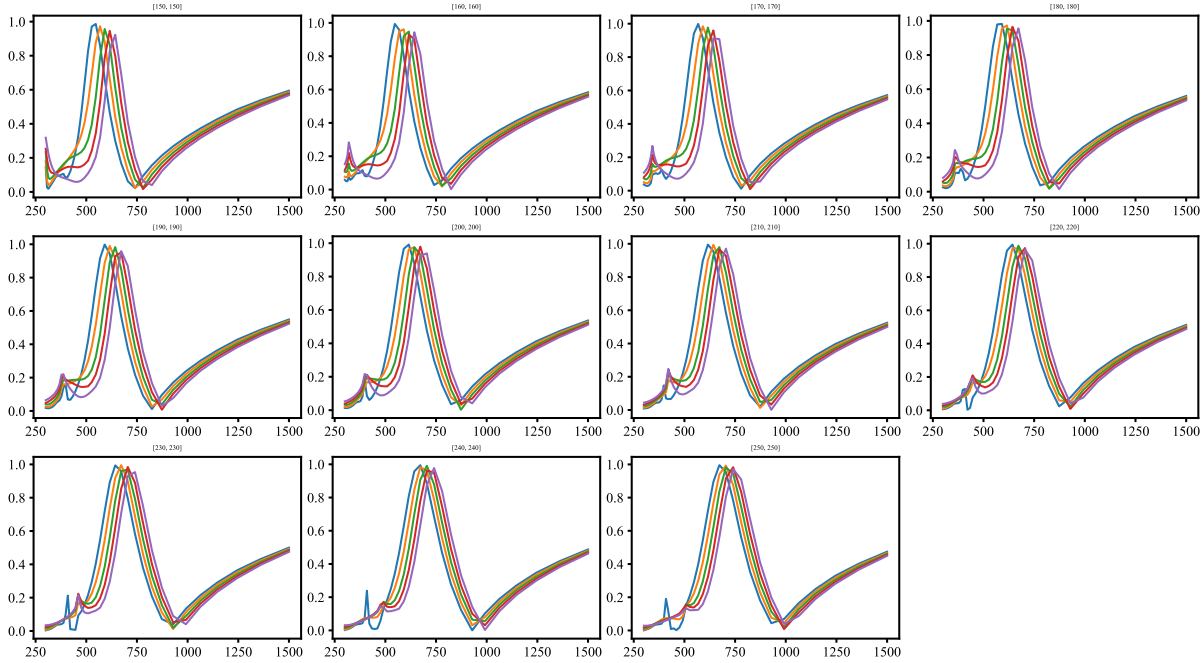

Figure S10. Polarization ratio of the transmitted light for the grating materials that contain 12% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

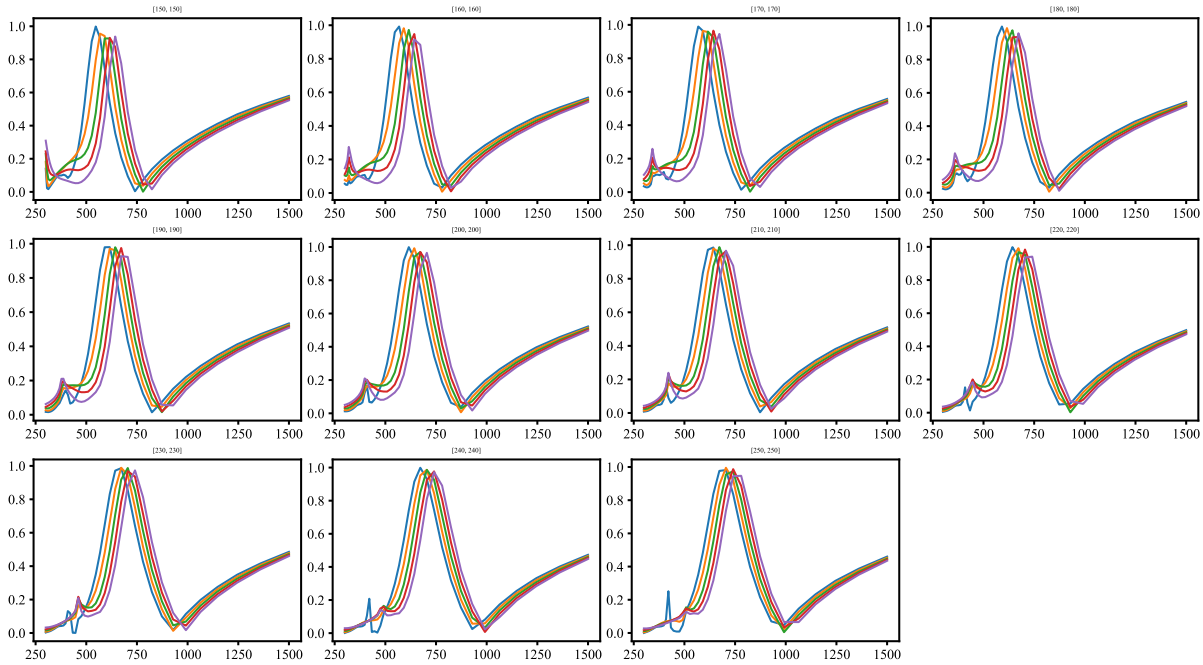

Figure S11. Polarization ratio of the transmitted light for the grating materials that contain 14% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

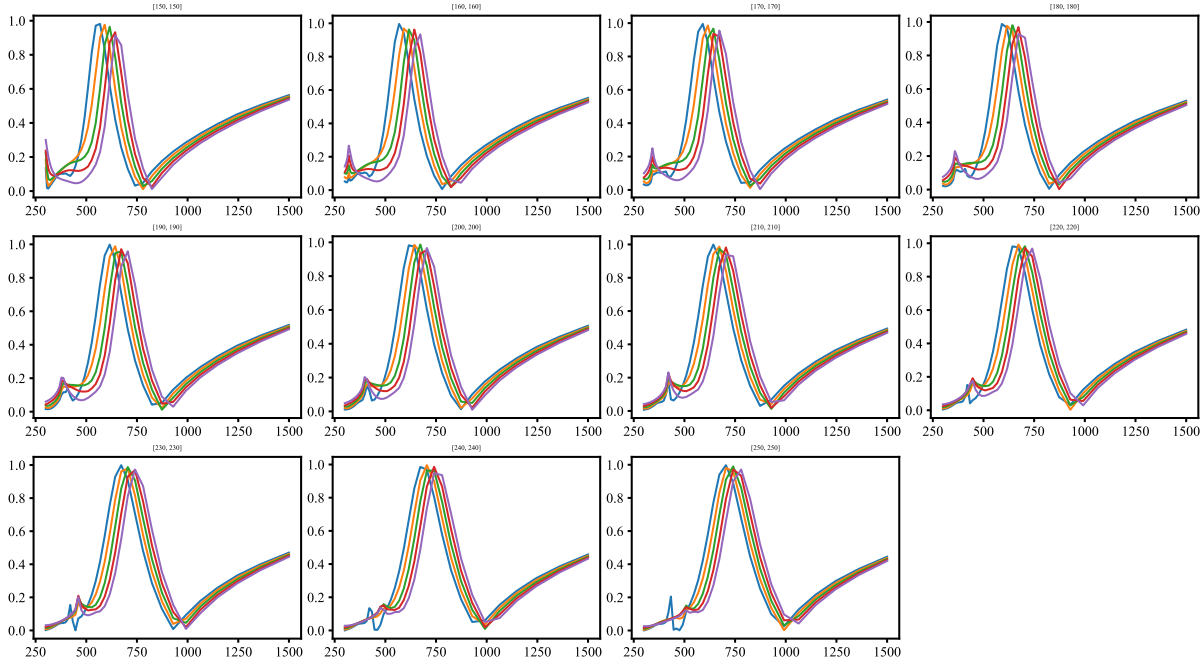

Figure S12. Polarization ratio of the transmitted light for the grating materials that contain 16% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

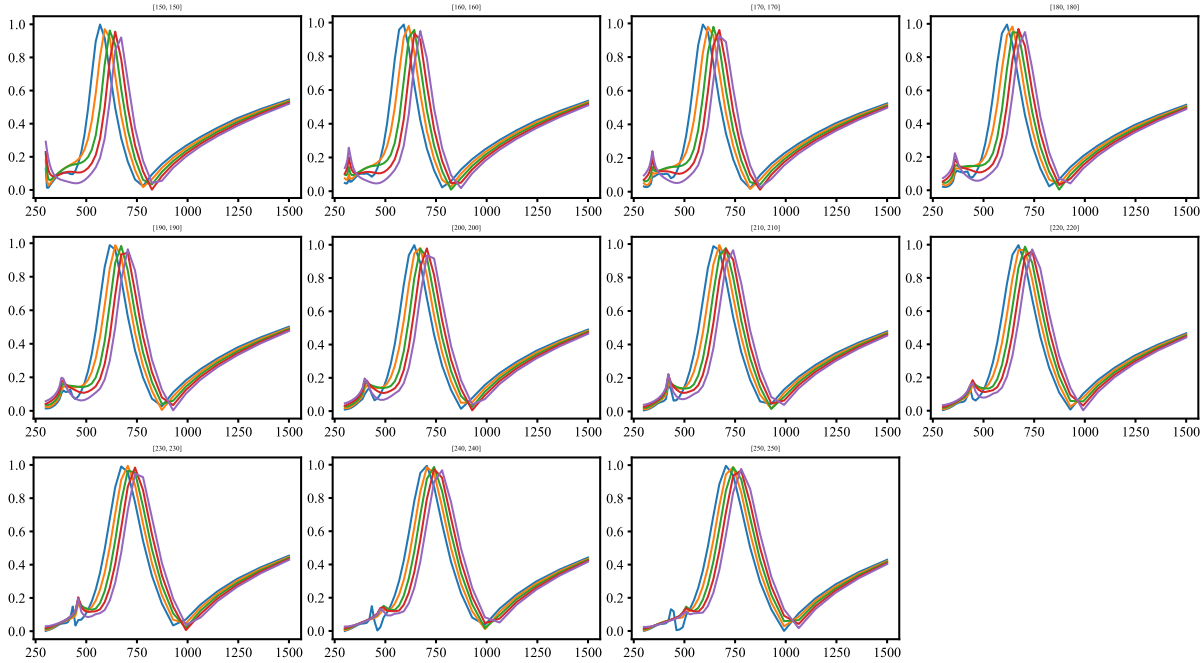

Figure S13. Polarization ratio of the transmitted light for the grating materials that contain 18% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

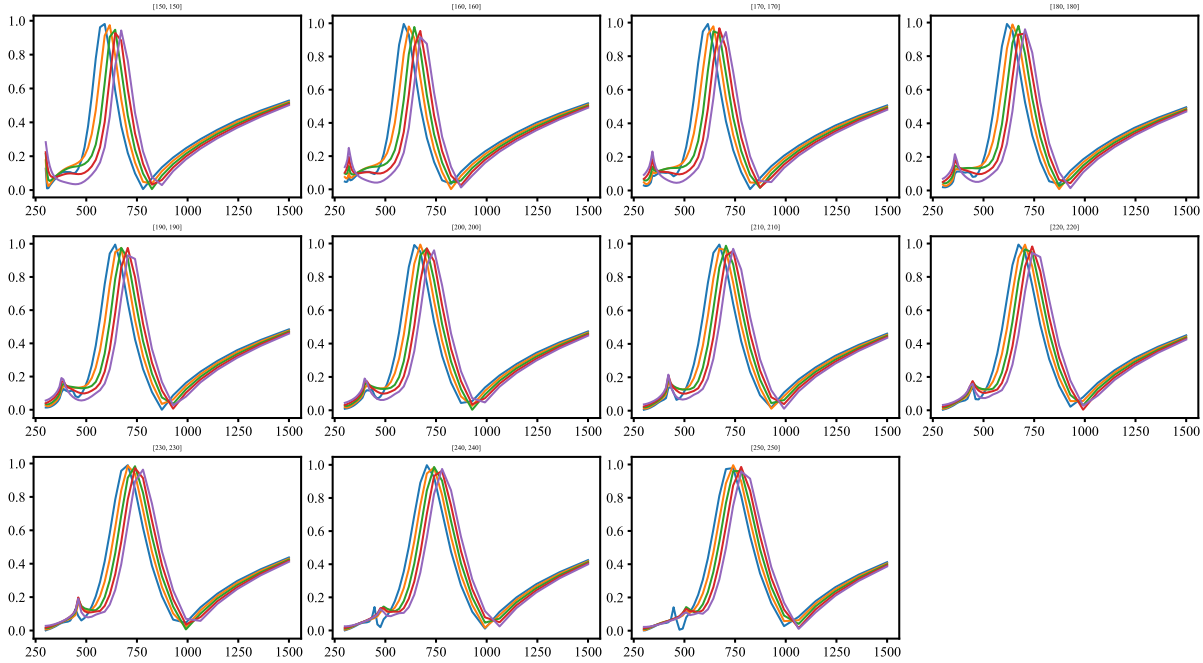

Figure S14. Polarization ratio of the transmitted light for the grating materials that contain 20% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

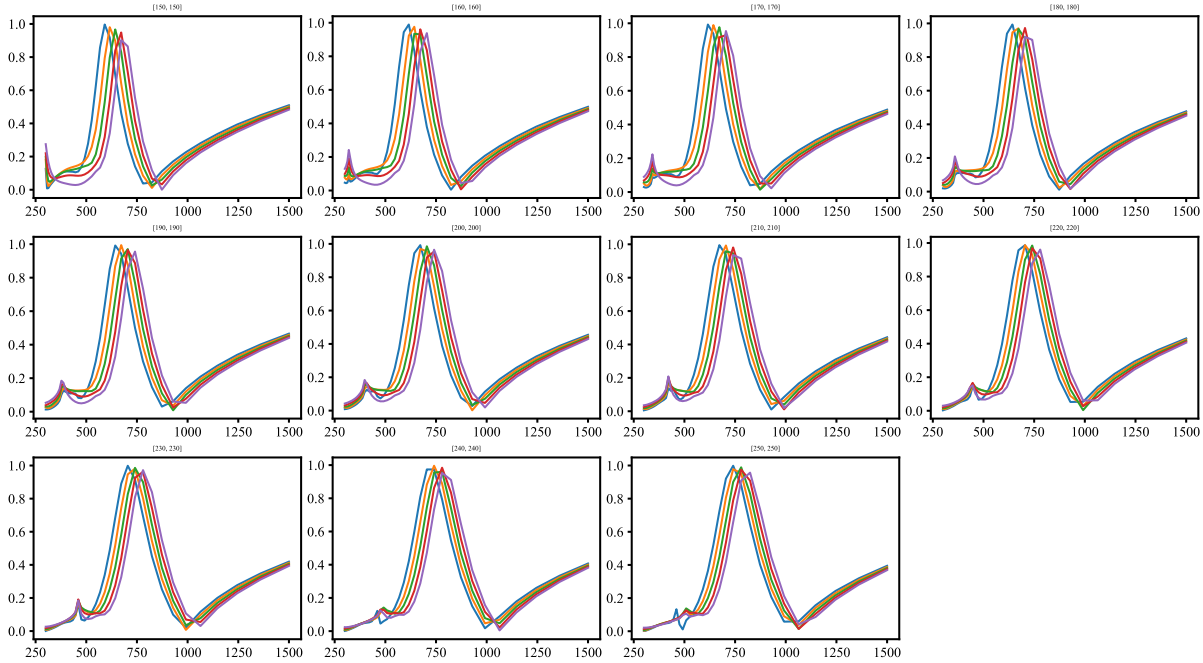

Figure S15. Polarization ratio of the transmitted light for the grating materials that contain 22% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

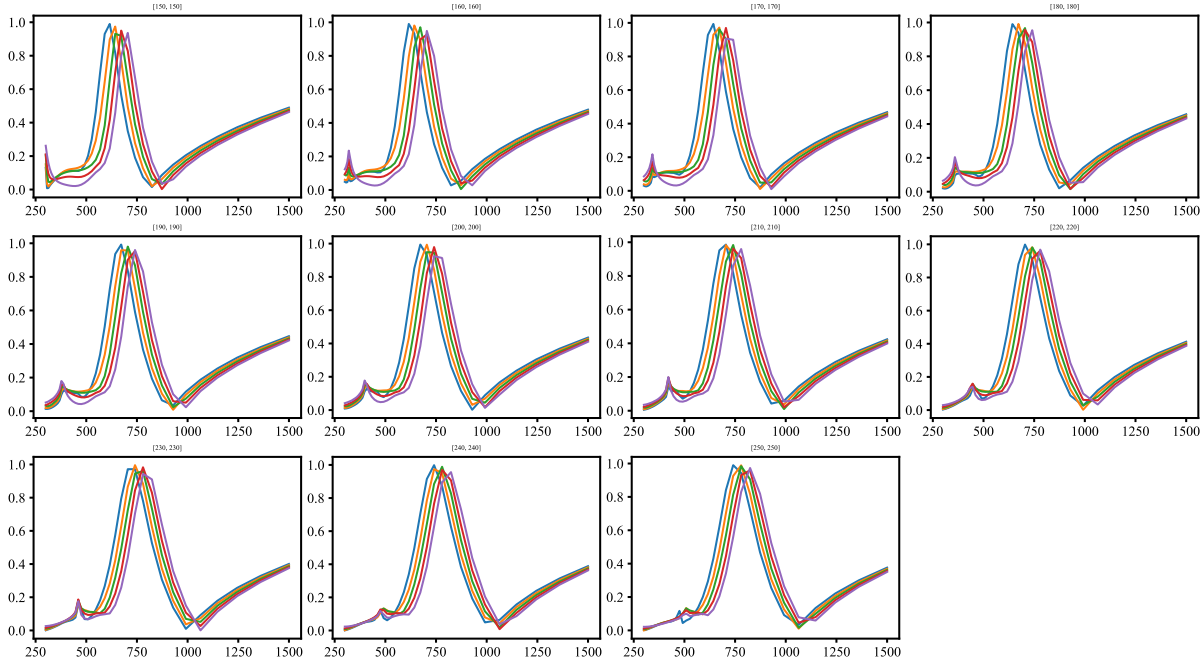

Figure S16. Polarization ratio of the transmitted light for the grating materials that contain 24% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

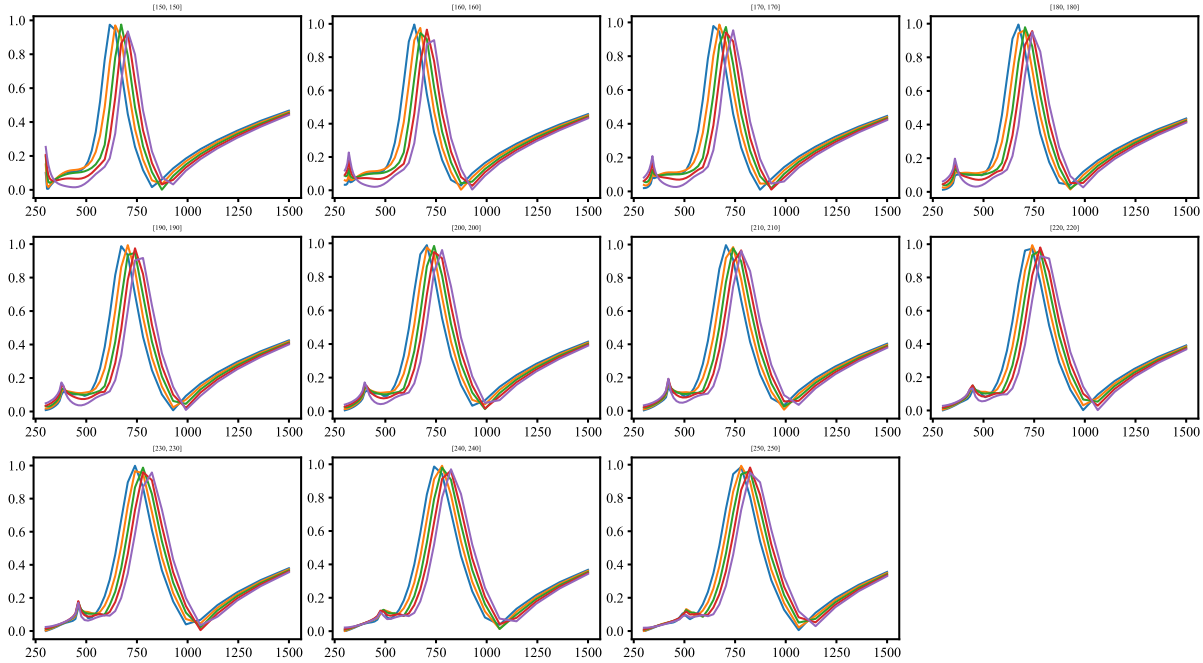

Figure S17. Polarization ratio of the transmitted light for the grating materials that contain 26% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

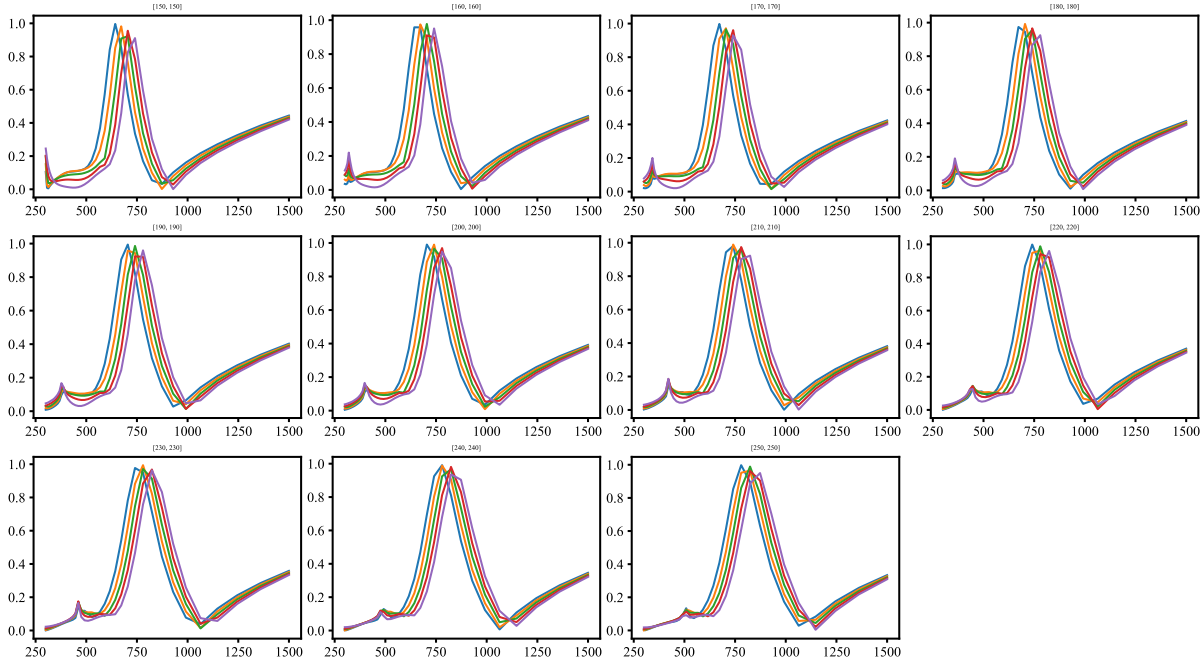

Figure S18. Polarization ratio of the transmitted light for the grating materials that contain 28% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

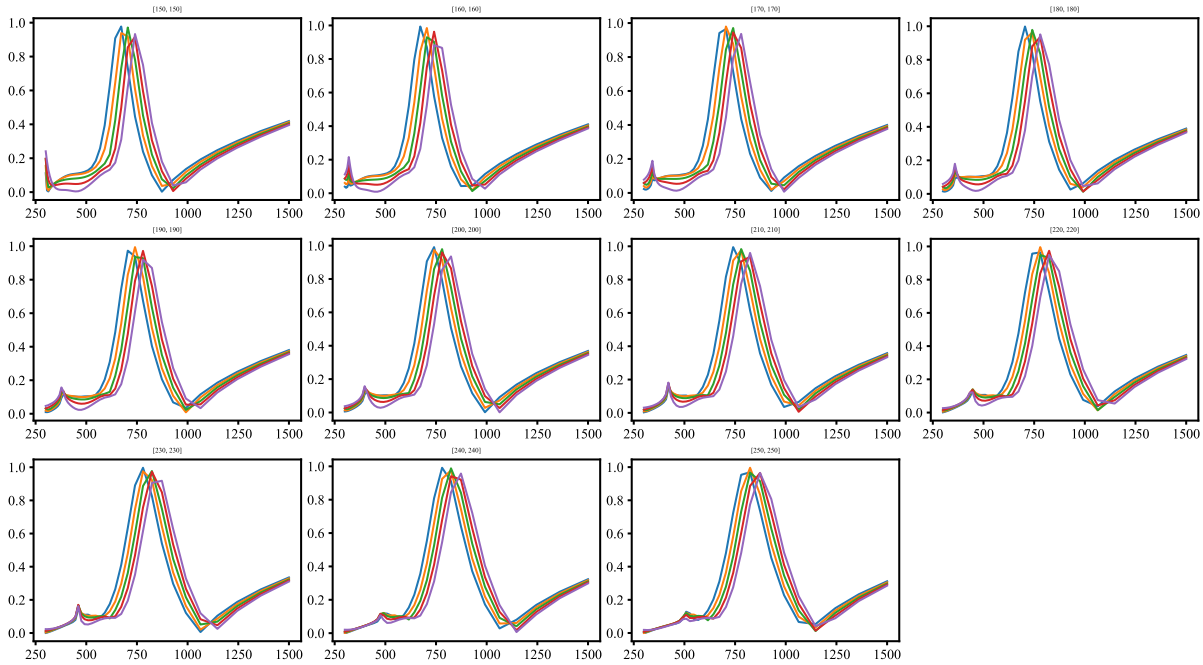

Figure S19. Polarization ratio of the transmitted light for the grating materials that contain 30% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

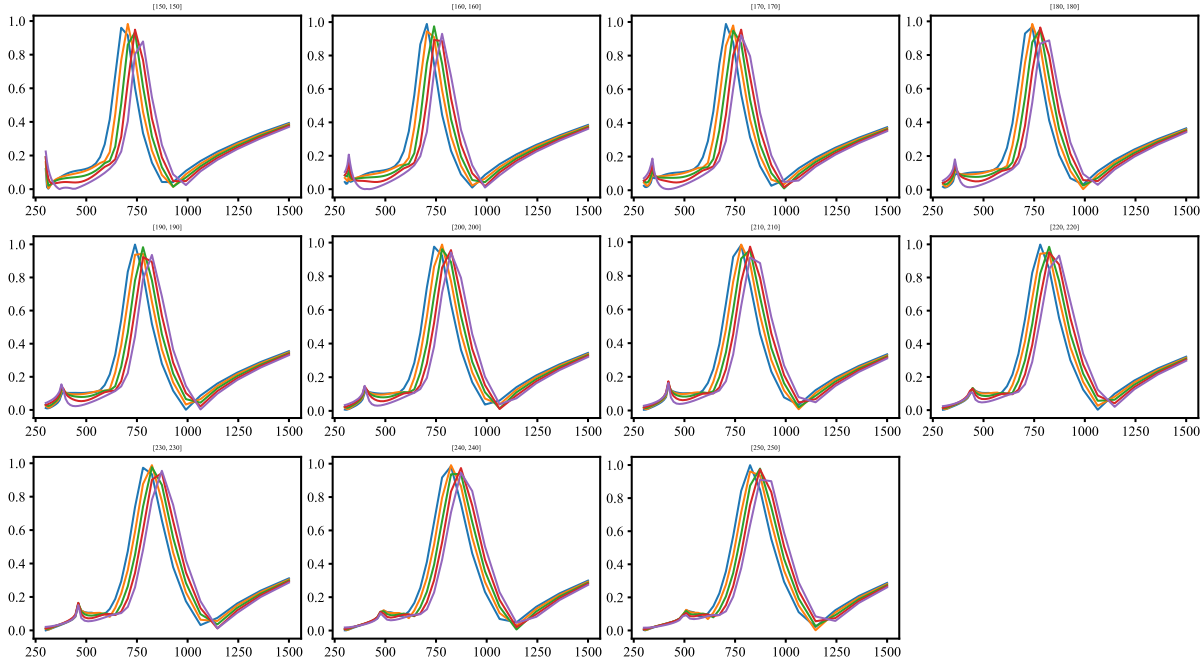

Figure S20. Polarization ratio of the transmitted light for the grating materials that contain 32% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

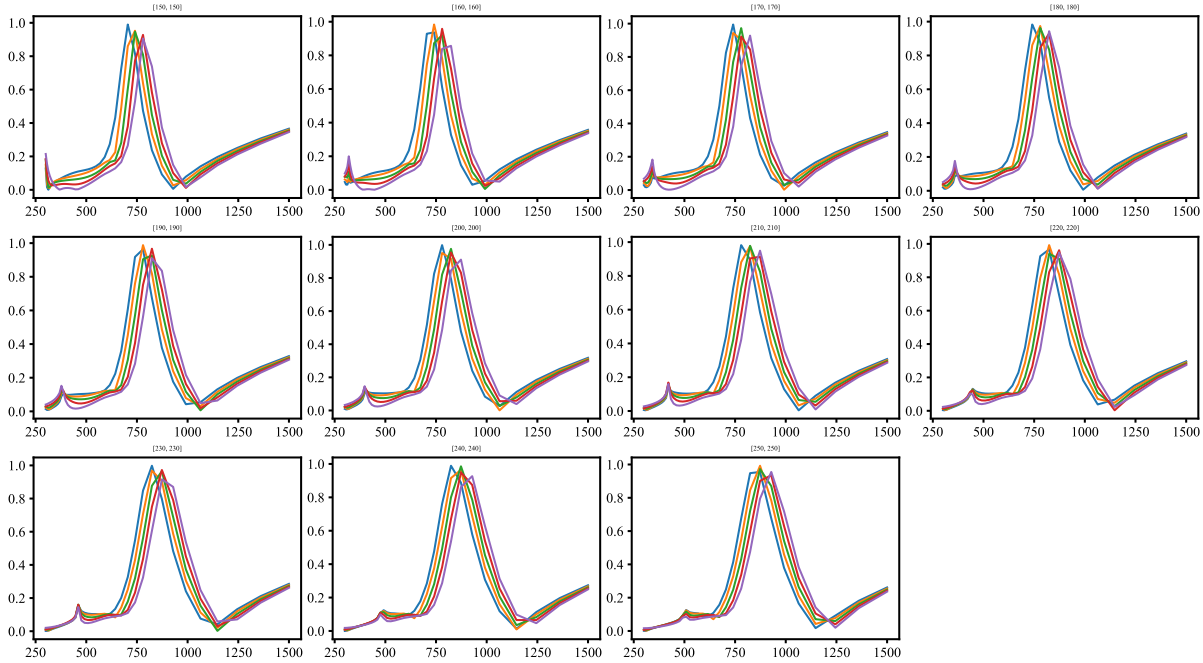

Figure S21. Polarization ratio of the transmitted light for the grating materials that contain 34% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

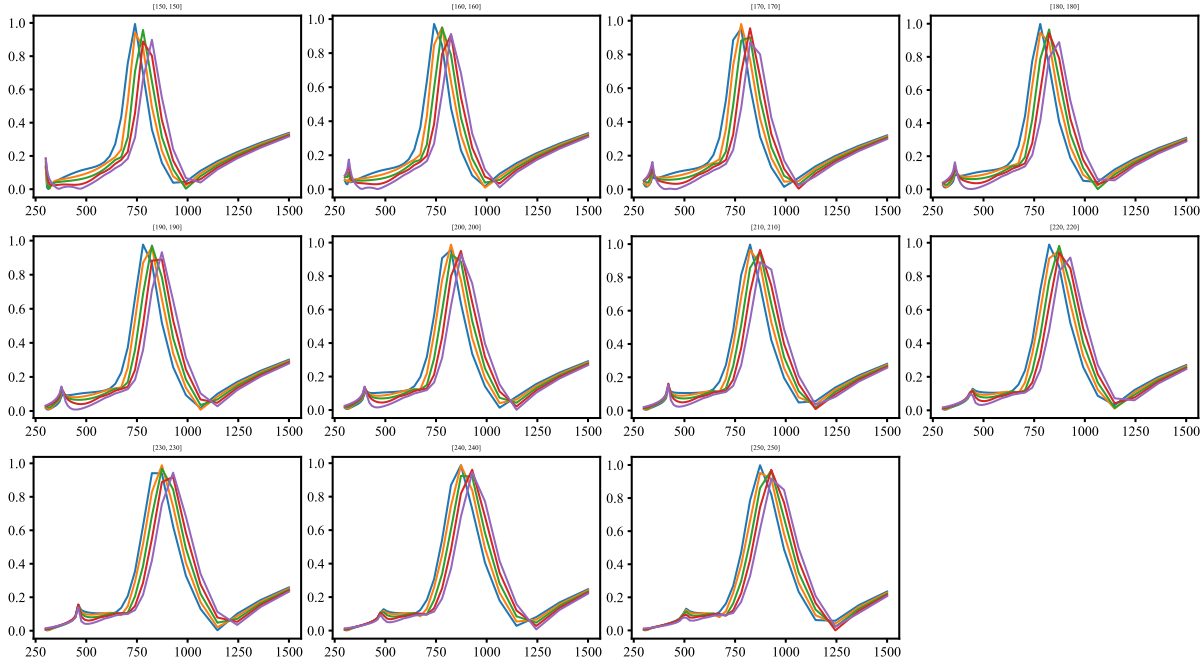

Figure S22. Polarization ratio of the transmitted light for the grating materials that contain 36% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

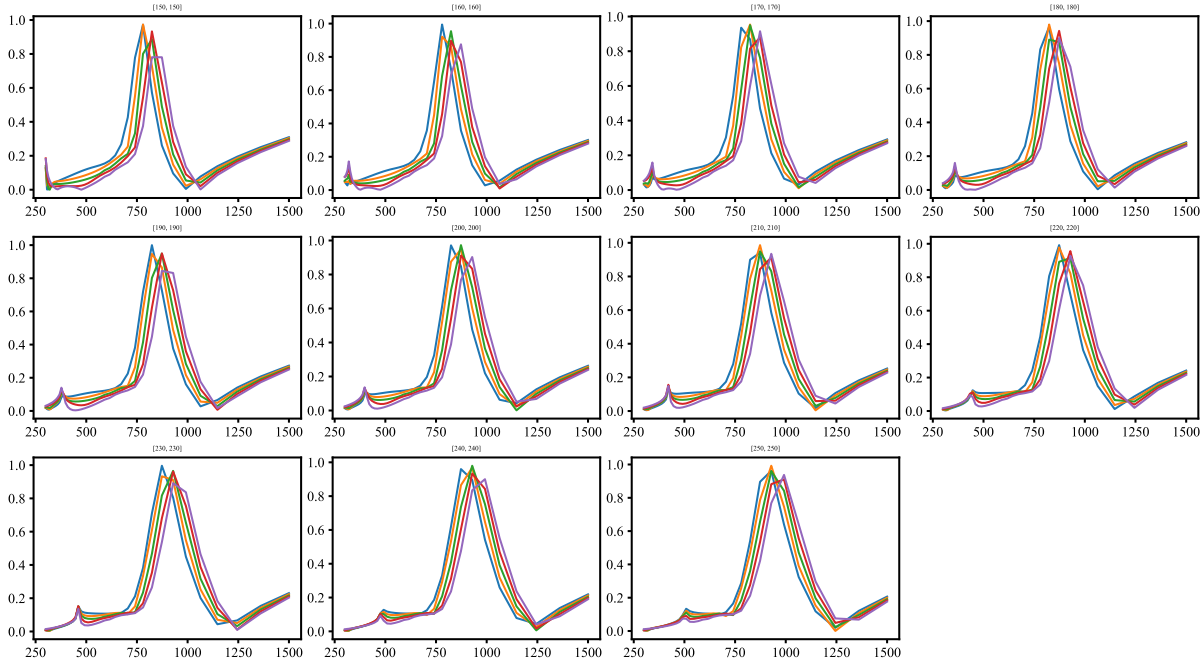

Figure S23. Polarization ratio of the transmitted light for the grating materials that contain 38% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

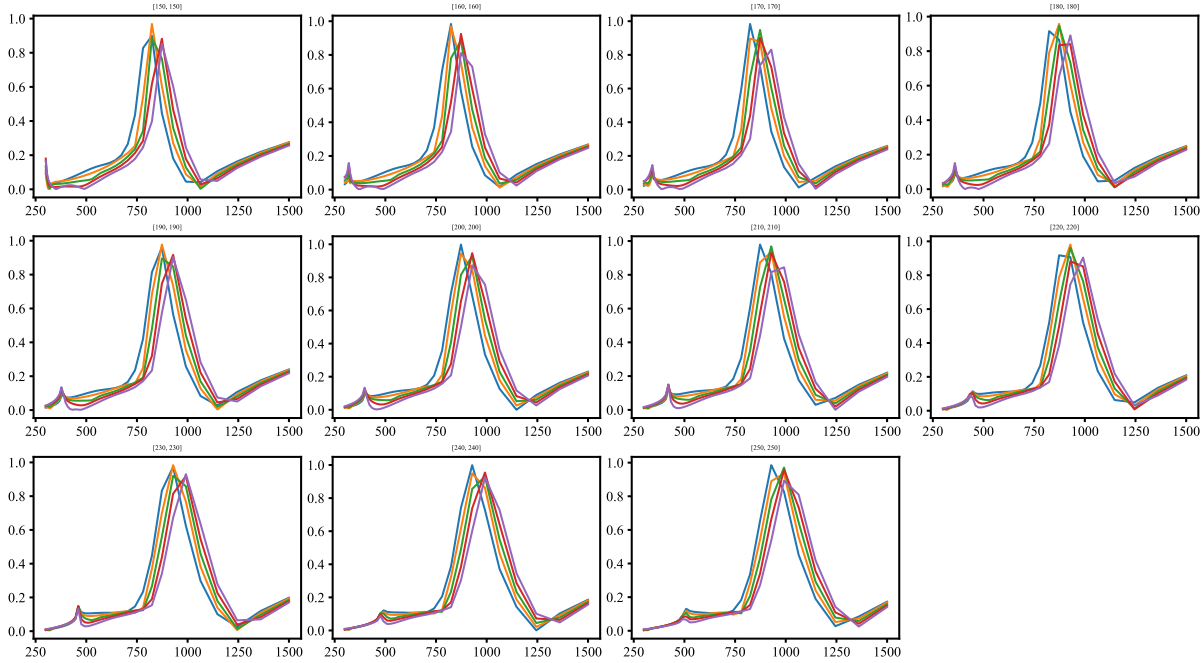

Figure S24. Polarization ratio of the transmitted light for the grating materials that contain 40% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

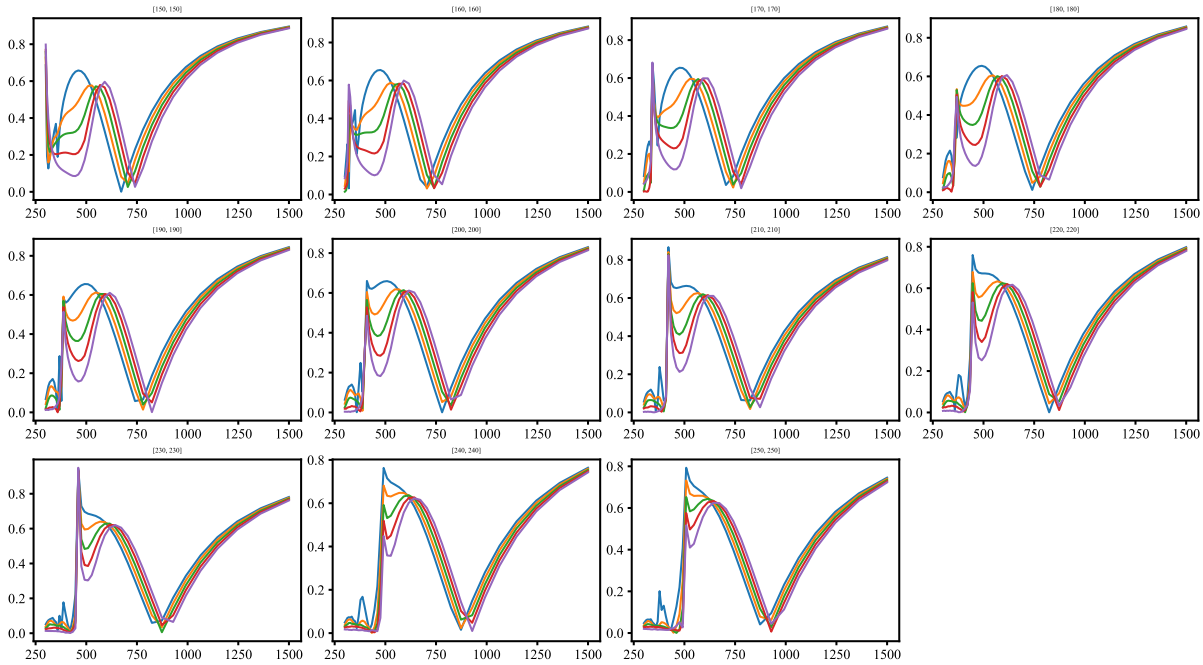

Figure S25. Polarization ratio of the reflected light for the grating materials that contain 0% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

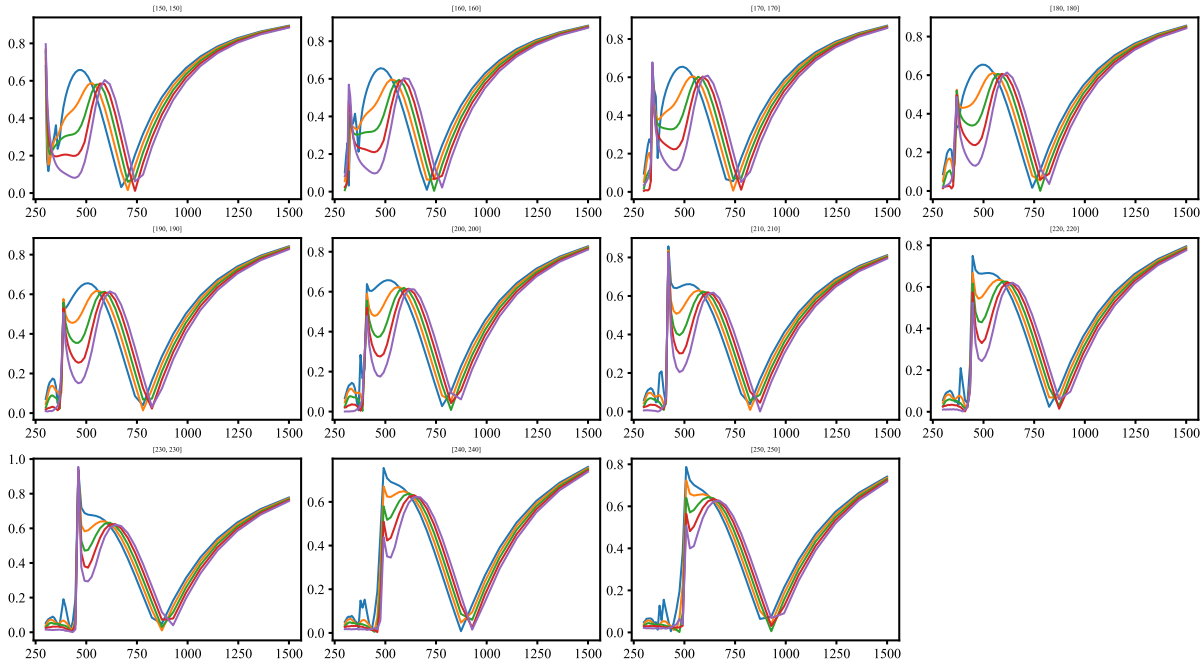

Figure S26. Polarization ratio of the reflected light for the grating materials that contain 2% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

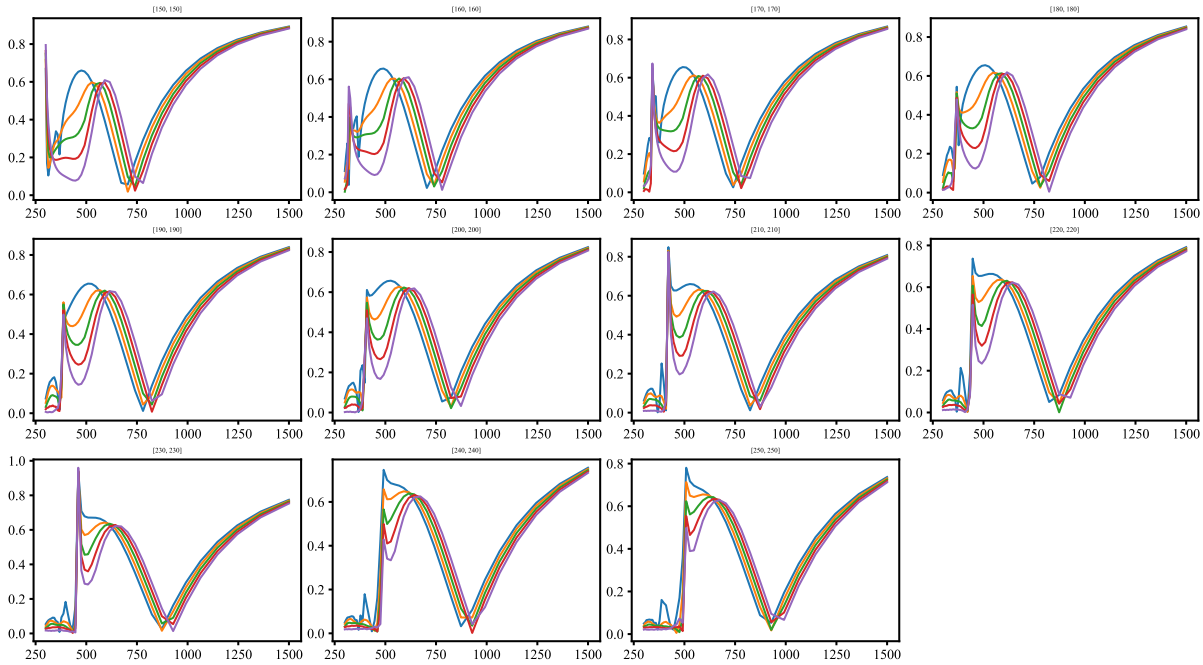

Figure S27. Polarization ratio of the reflected light for the grating materials that contain 4% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

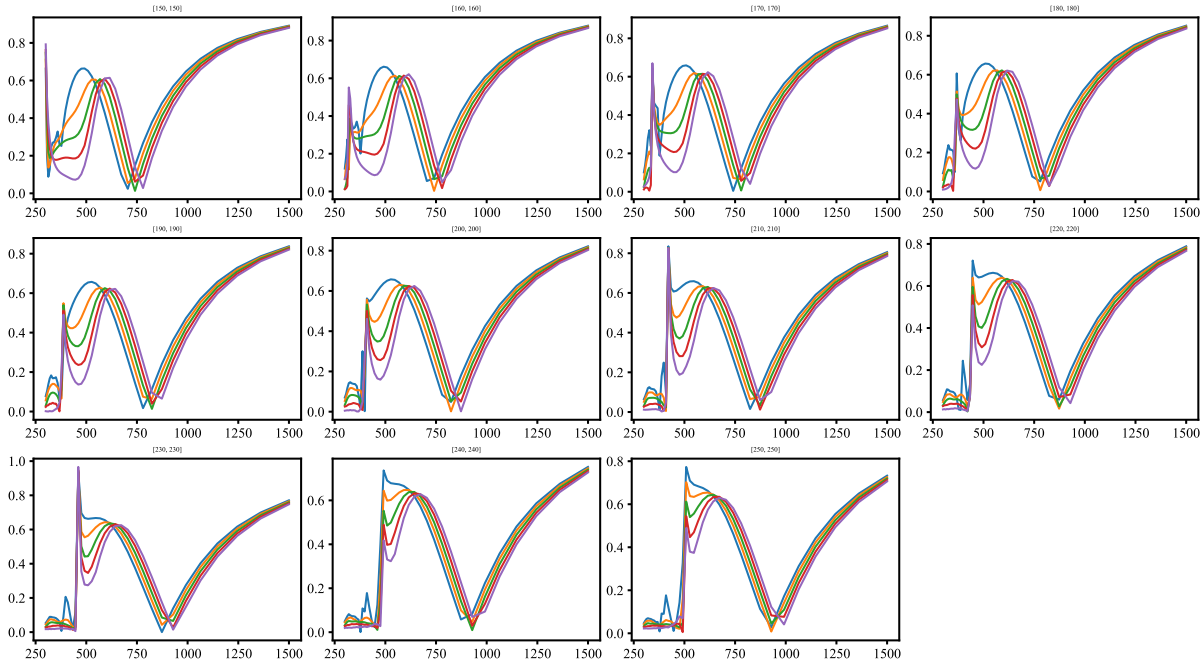

Figure S28. Polarization ratio of the reflected light for the grating materials that contain 6% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

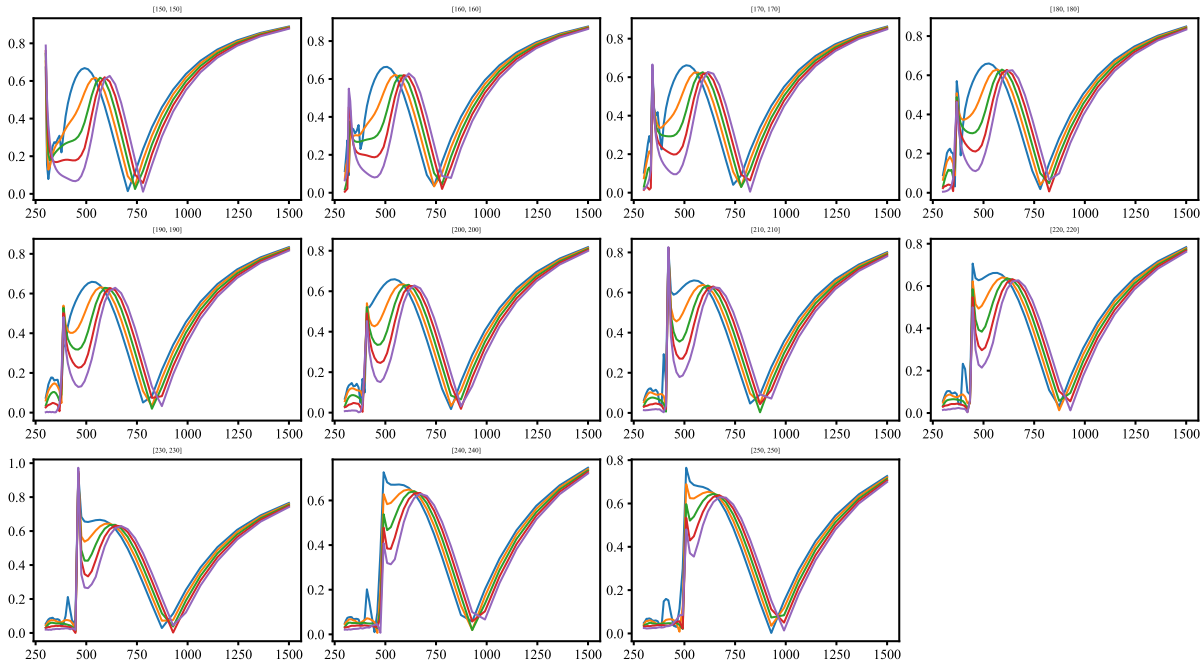

Figure S29. Polarization ratio of the reflected light for the grating materials that contain 8% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

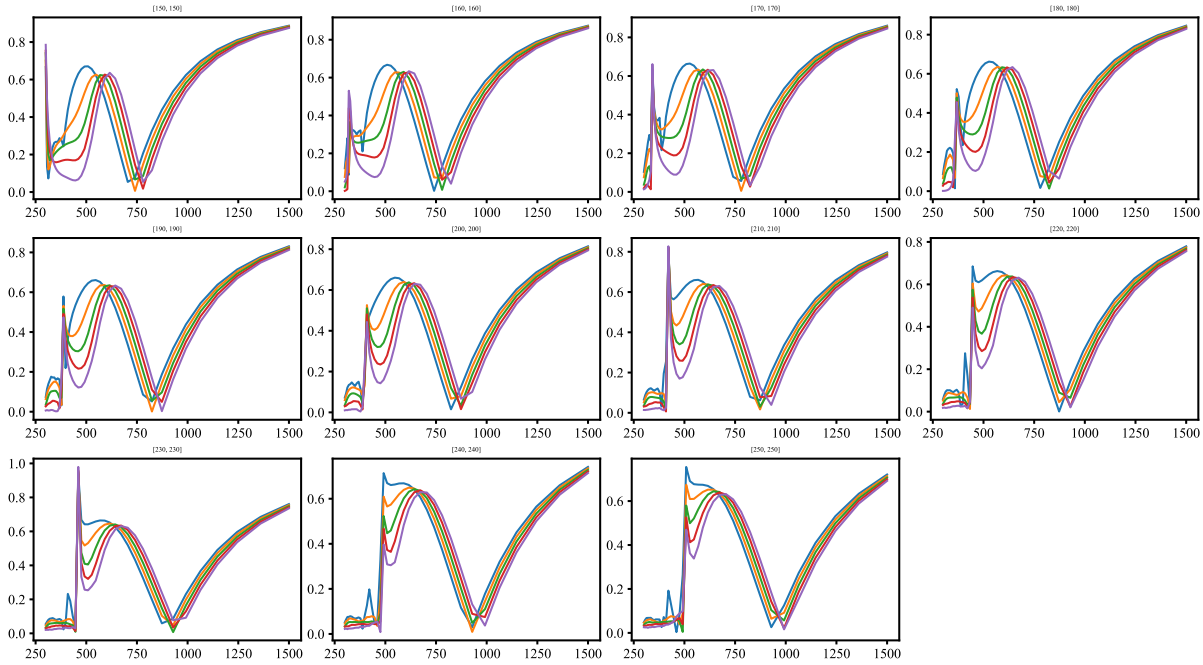

Figure S30. Polarization ratio of the reflected light for the grating materials that contain 10% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

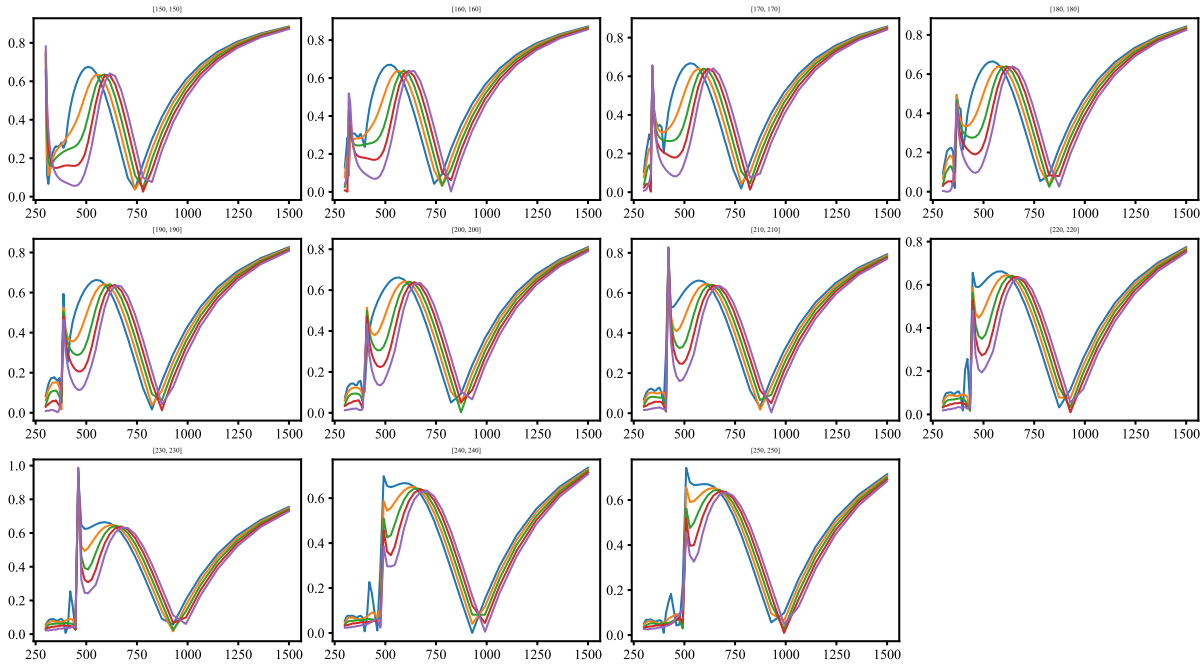

Figure S31. Polarization ratio of the reflected light for the grating materials that contain 12% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

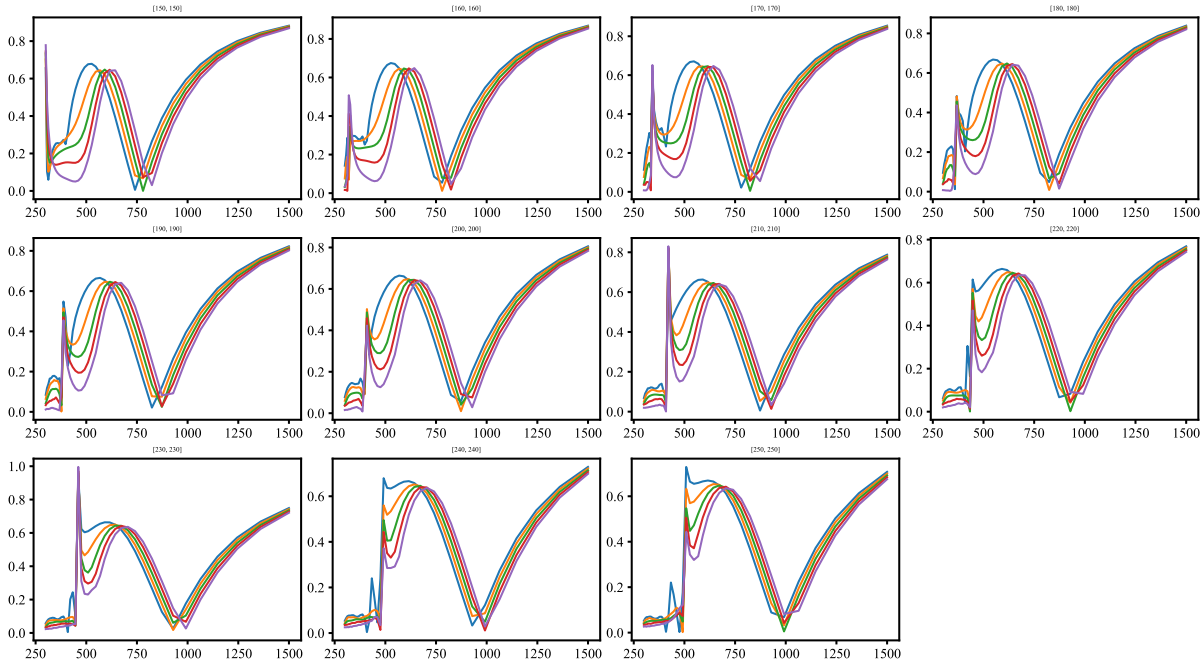

Figure S32. Polarization ratio of the reflected light for the grating materials that contain 14% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

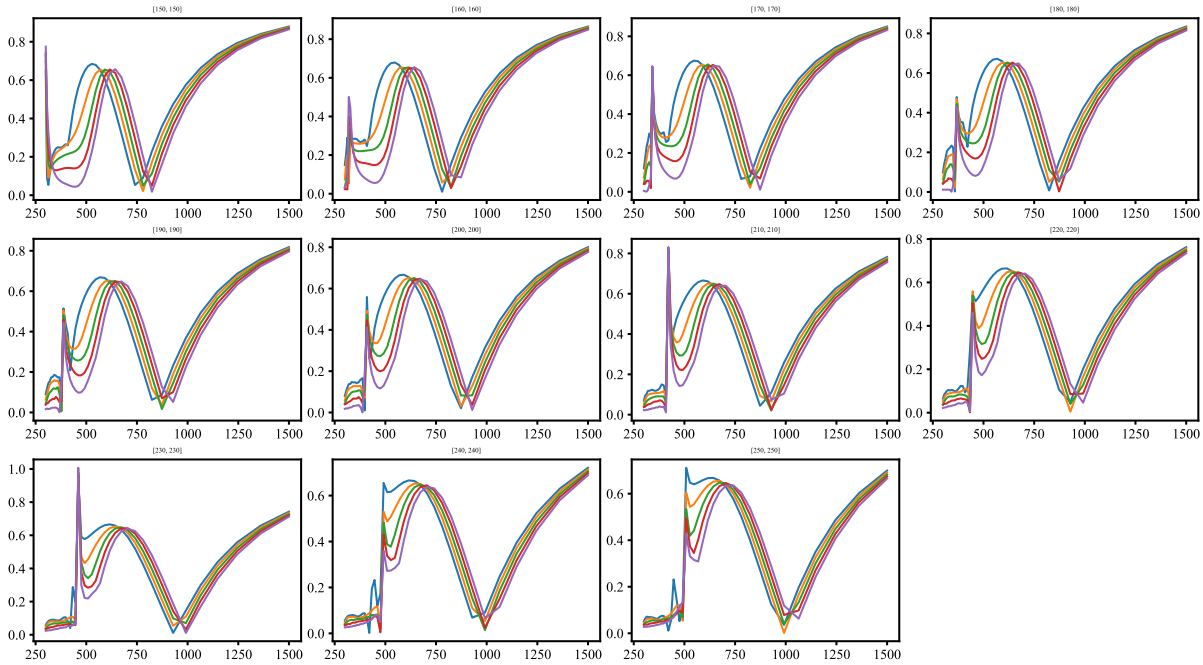

Figure S33. Polarization ratio of the reflected light for the grating materials that contain 16% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

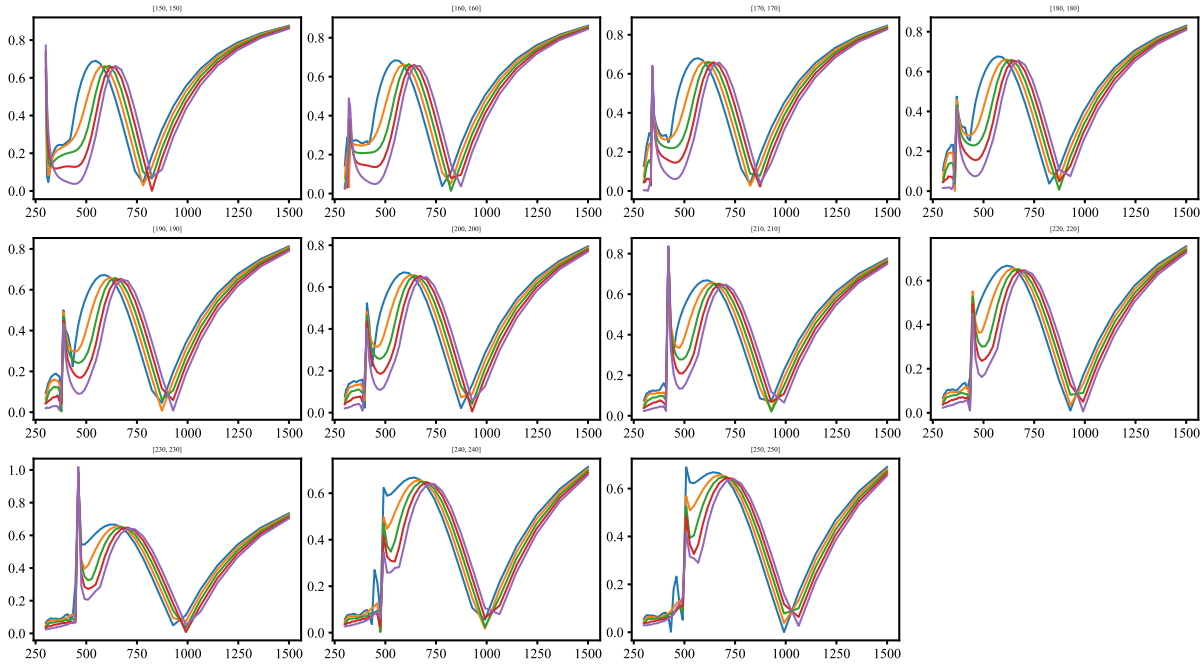

Figure S34. Polarization ratio of the reflected light for the grating materials that contain 18% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

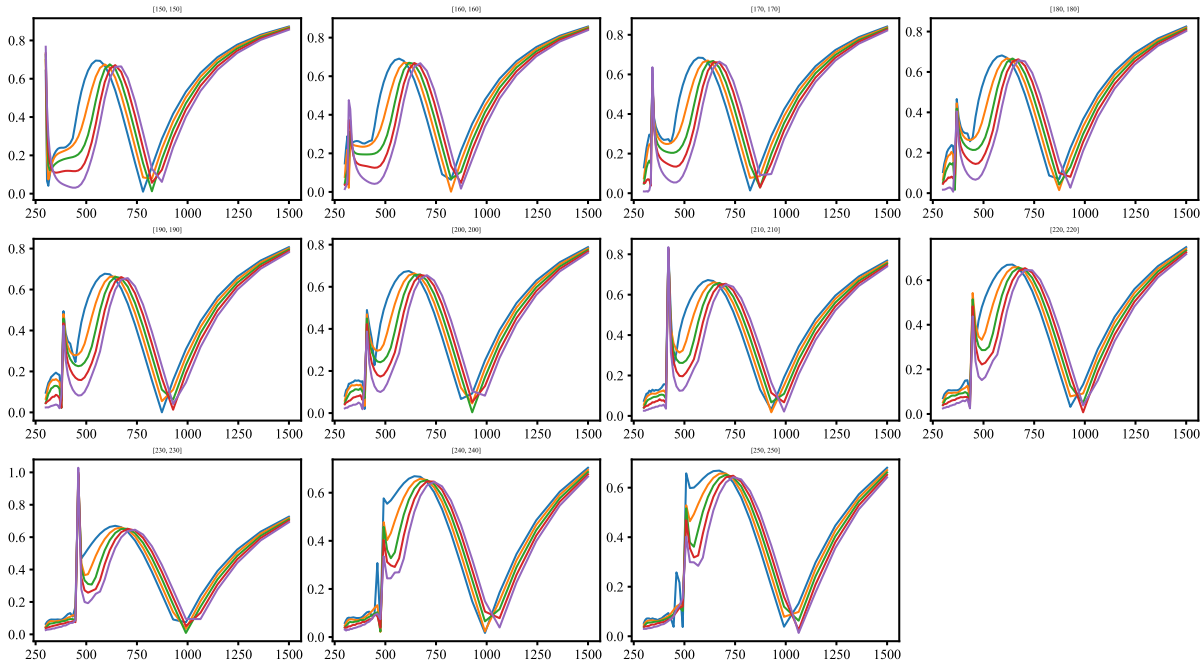

Figure S35. Polarization ratio of the reflected light for the grating materials that contain 20% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

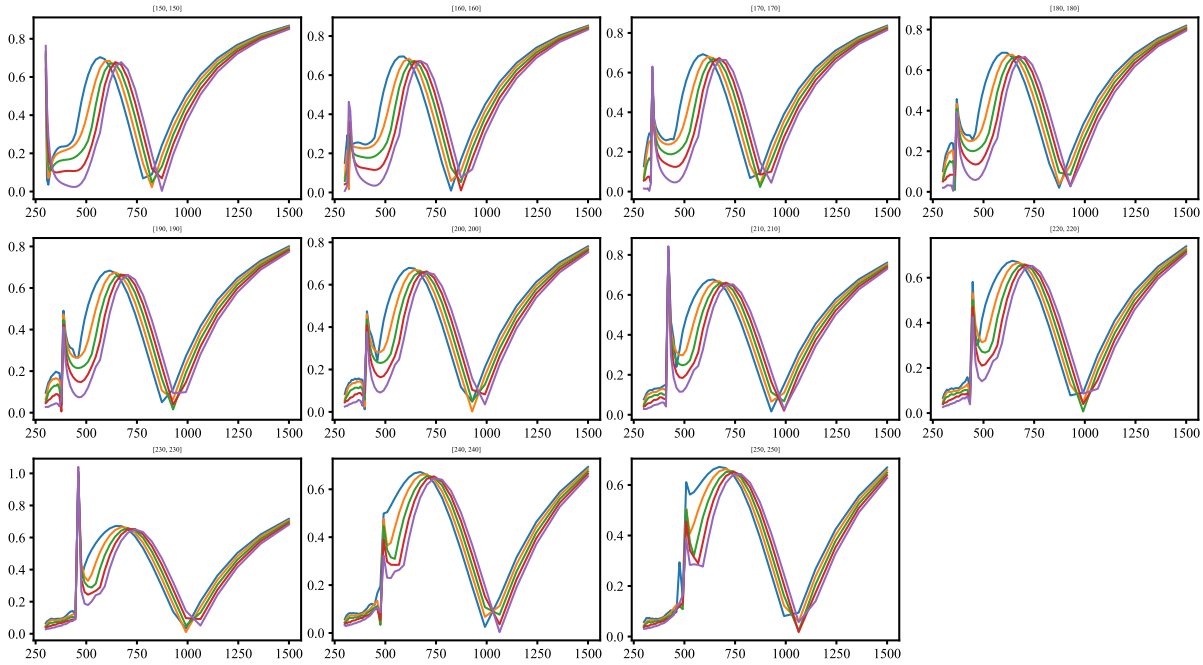

Figure S36. Polarization ratio of the reflected light for the grating materials that contain 22% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

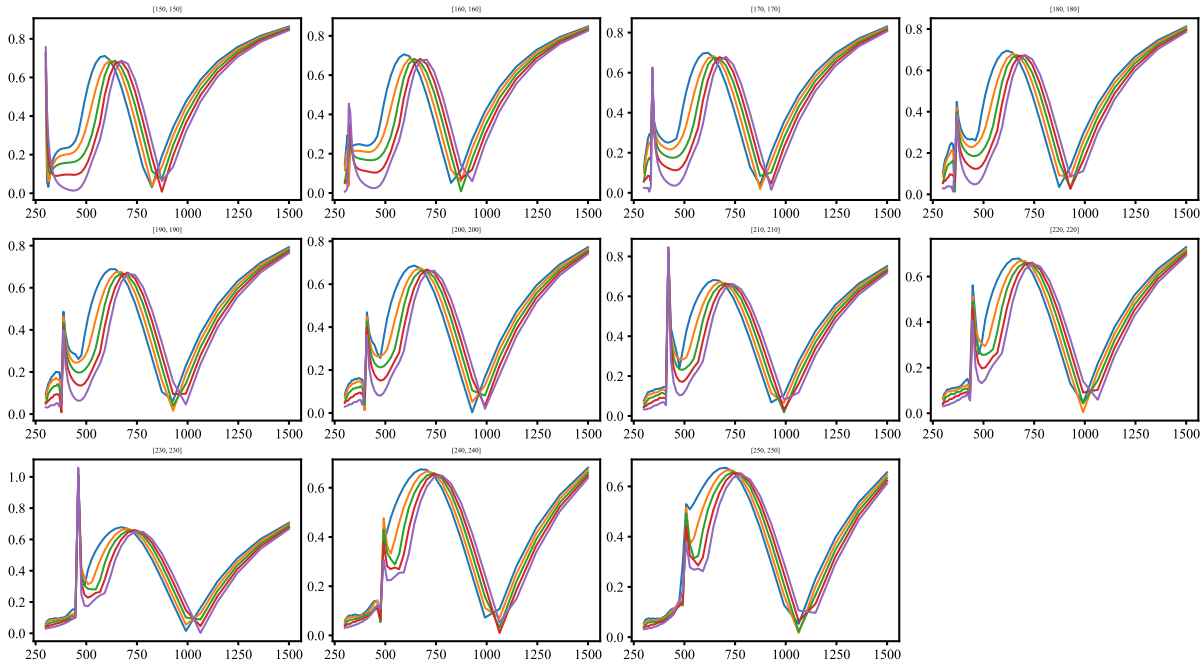

Figure S37. Polarization ratio of the reflected light for the grating materials that contain 24% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

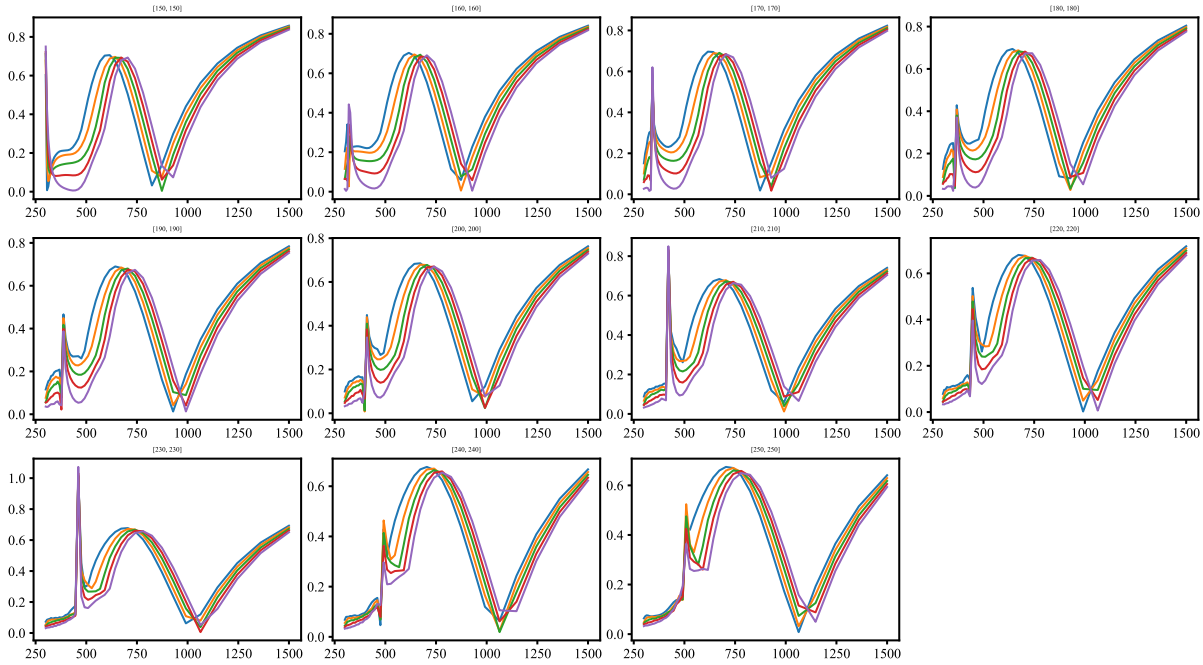

Figure S38. Polarization ratio of the reflected light for the grating materials that contain 26% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

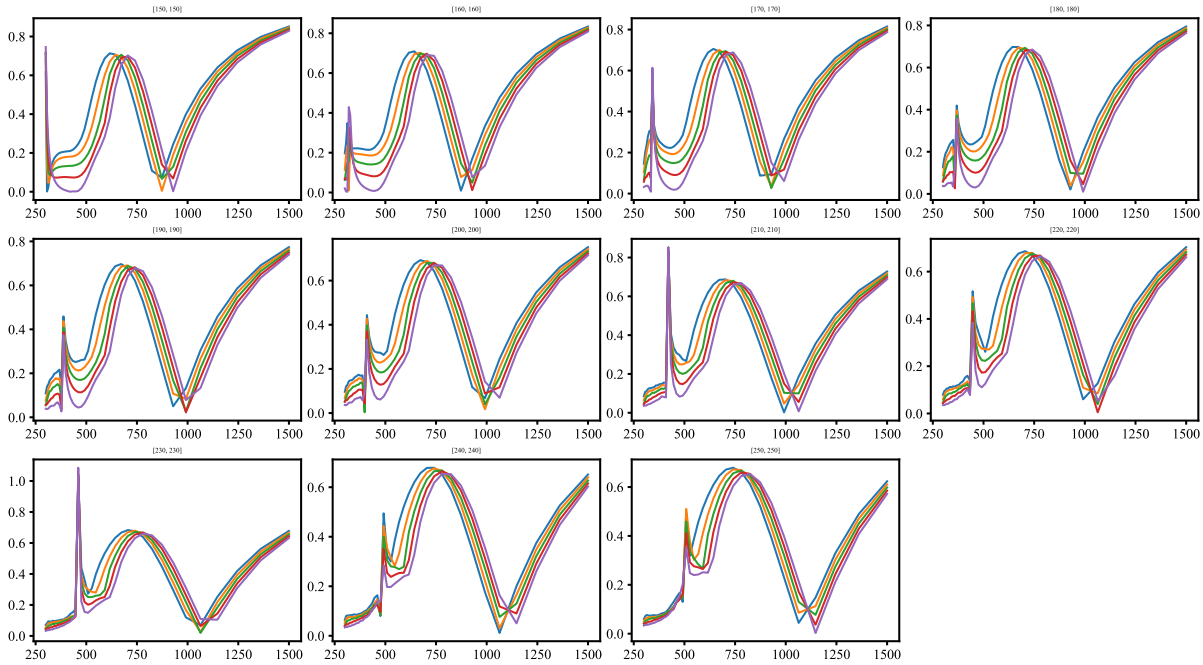

Figure S39. Polarization ratio of the reflected light for the grating materials that contain 28% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

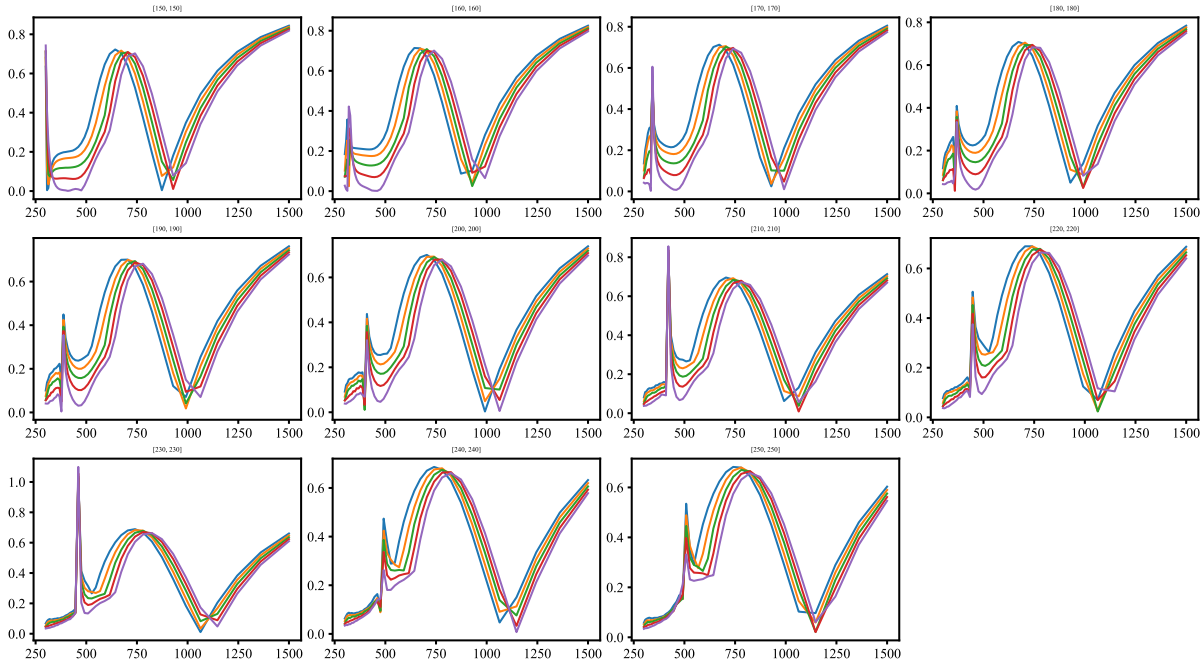

Figure S40. Polarization ratio of the reflected light for the grating materials that contain 30% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

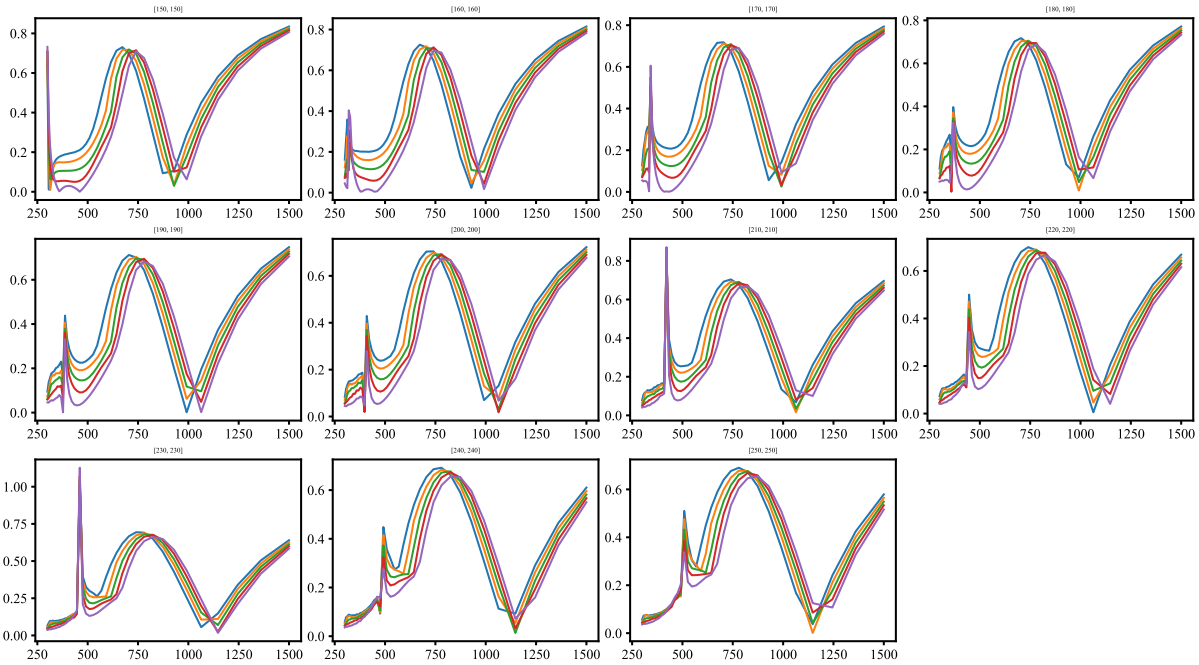

Figure S41. Polarization ratio of the reflected light for the grating materials that contain 32% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

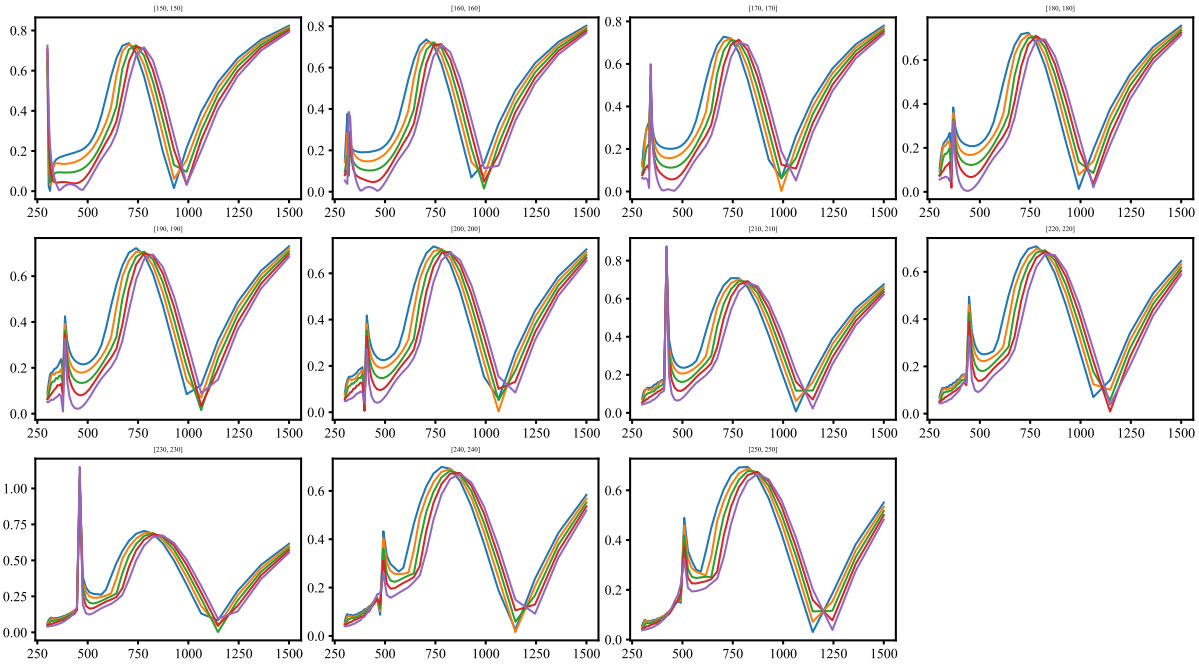

Figure S42. Polarization ratio of the reflected light for the grating materials that contain 34% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

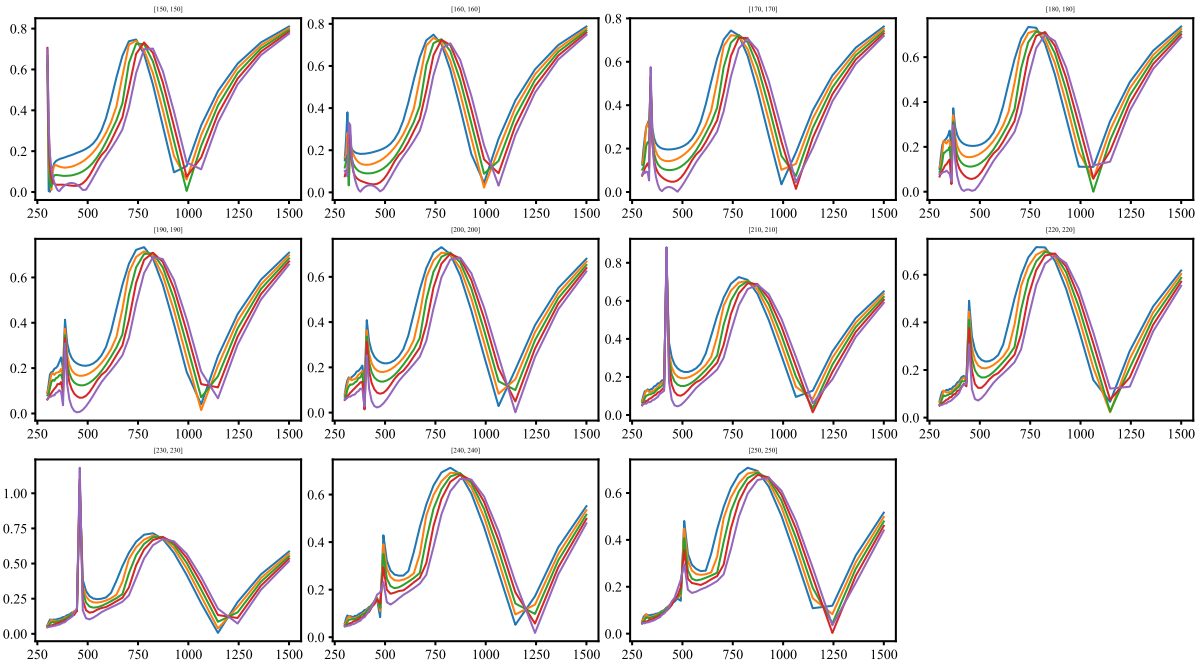

Figure S43. Polarization ratio of the reflected light for the grating materials that contain 36% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

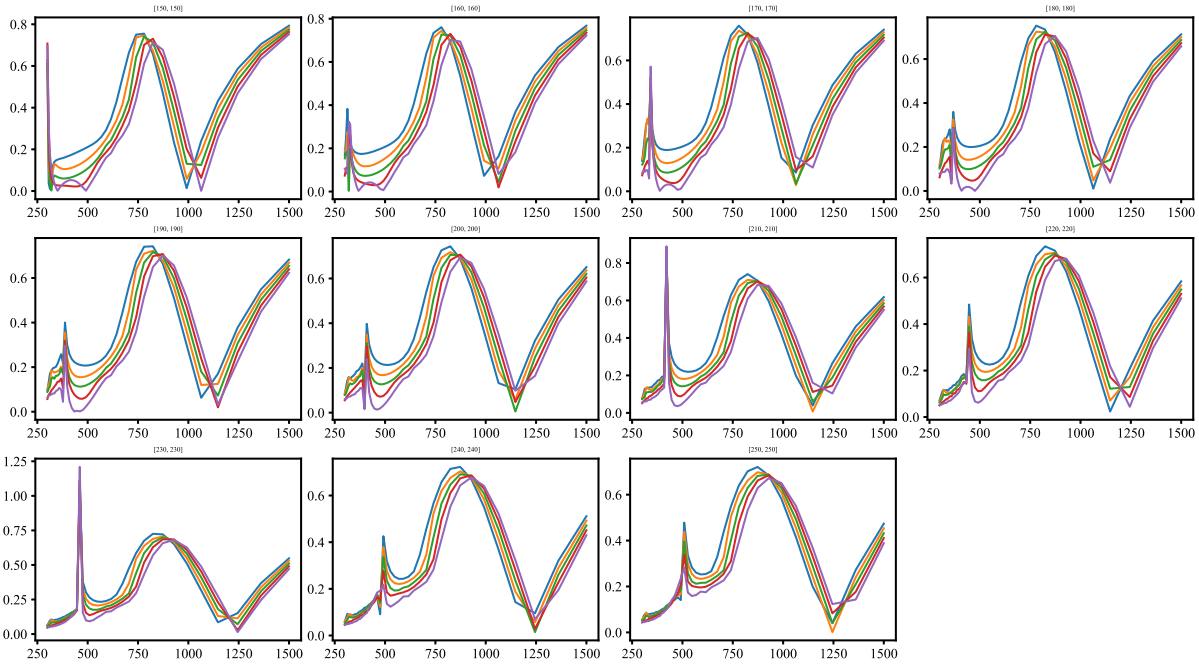

Figure S44. Polarization ratio of the reflected light for the grating materials that contain 38% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.

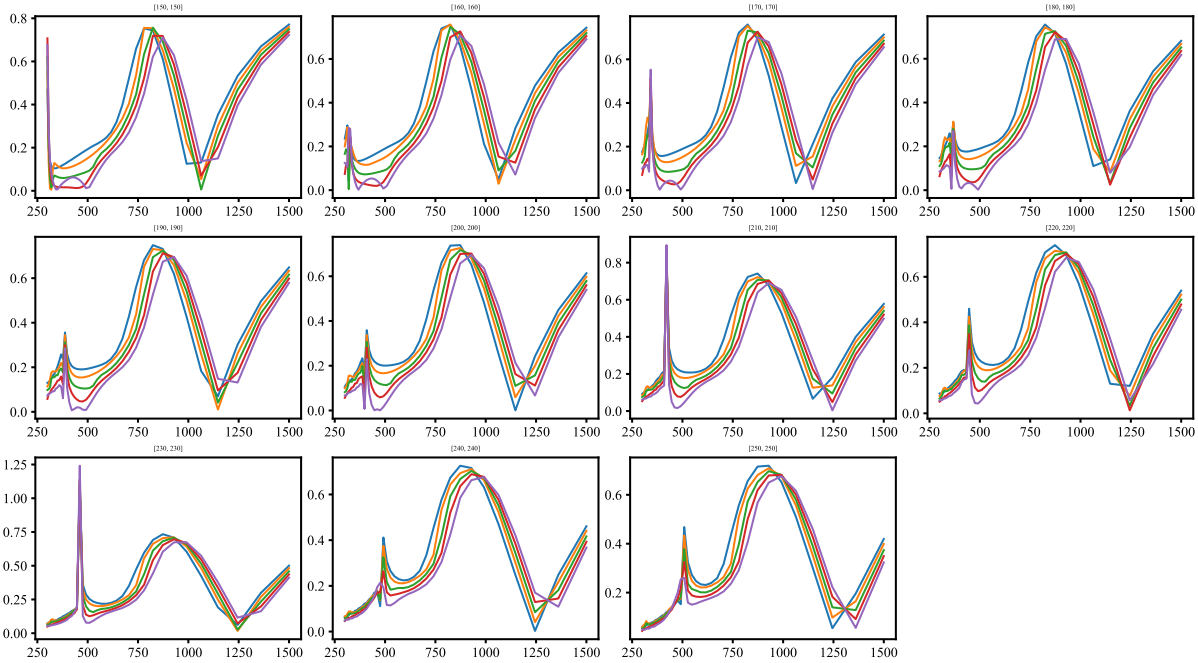

Figure S45. Polarization ratio of the reflected light for the grating materials that contain 40% PDMS. The subtitle of each subfigure represents W, and distance between gratings (G-W) (see Figure 1 in the main text). Blue, orange, green, red, and purple lines represent 0:1, 1:3, 1:1, 3:1, and 1:0 gold:silver relative concentration ratios of the grating material, respectively.