Usage Report for Fiscal Year 2022

Project Title:

Electric field and molecular analysis for plasmonic gas sensors

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1. Background and purpose of the project, relationship of the project with other projects

We are now developing three-dimensional plasmonic gas sensors that are metallic nanometer-sized double fin structures to sense the presence of volatile organic compounds, such as benzene, formaldehyde and toluene. To efficiently detect these dangerous molecules, however, the resonance frequency of the plasmonic sensor should overlap with the vibrational absorption frequency of the target molecule. Hence, tailoring the optical response of the plasmonic gas sensor for specific target gas molecules is needed. In this project, we explore the optical properties of our double fin plasmonic gas sensor, particularly, how each part of the gas sensor's structure affects the optical response of the sensor.

2. Specific usage status of the system and calculation method

In the course of FY2022, we have used HOKUSAI as a vehicle to simulate the optical response of our plasmonic gas sensor, focusing on the transmission, reflection and absorption spectra, through an open-source software called Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience (SALMON). Using SALMON, we conducted finite-difference time-domain (FDTD) calculations using a double fin/grating model. The electric field is introduced normal to the surface of the model and polarized along the short axis of the structure. The target resonance frequency of the structure is around 2965 cm^{-1} that is the absorption peak for butane gas, our experimental test sample.

3. Results and Conclusion

Our double fin plasmonic gas sensor is comprised of two vertical Au fins with some residual SiO_2 in between and this entire structure is anchored on a Si grating. We conducted two sets of FDTD simulations: (1) the Si grating only and (2) the Si grating with the Au-SiO_2 vertical structures. For (1), we found that the Si grating alone has peaks around 7691 cm^{-1} and 4761 cm^{-1}. These peaks are shifted to lower frequencies when the Au-SiO_2 structures are included in the model. For (2), we found two new resonance peaks around 3332 cm^{-1} and 3076 cm^{-1}, that we attribute to the double fin structure. When we increased the Si grating width from 1.0 μm to 1.6 μm, the 3076 cm^{-1} shifts to lower frequencies (2318 cm^{-1} for 1.6 μm). This opens an avenue for possible tunability of our proposed plasmonic gas sensor structure. It is still yet to be determined if the shifting secondary peak at 3076 cm^{-1} is primarily due to the individual double fin structure or due to its interaction with neighboring double fin structures since their proximity increases as the grating width increases.

4. Schedule and prospect for the future

There are still many variables that need to be considered, such as the Au fin height and the SiO_2 depth, and how they affect the overall resonance of the plasmonic structure. The angle of incidence of the illuminating electric field must also be explored to fully replicate the current experimental setup. For FY2023, I would like to focus on the aforementioned simulations and, therefore, would like to continue using HOKUSAI.