Usage Report for Fiscal Year 2023

Project Title:

Electric field and molecular analysis for plasmonic gas sensors

Name:
○Maria Vanessa Balois Oguchi

Laboratory at RIKEN:
Innovative Photon Manipulation Research Team, RIKEN Center for Advanced Photonics

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

Related to our FY2022: Q22581 project, we are continuing to develop three-dimensional plasmonic gas sensors that use metallic double fin nanostructures that utilize the metal-insulator-metal (MIM) configuration to detect gas molecules. In order for efficient detection to occur, the resonance frequency of the MIM plasmonic sensor must be engineered to be the same as the vibrational absorption frequency of the molecule. For this project, we aimed to model both the optical properties and electromagnetic field distribution of our MIM plasmonic nanostructure.

2. Specific usage status of the system and calculation method

We intended to continue performing finite difference time domain calculations (FDTD) for our double fin/grating model that we developed last year (FY2022: Q22581) using the open-source software called Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience (SALMON). However, after implementing the experiment, we determined that oblique angle of incidence was necessary. As a result, it was necessary to revise our previous simulation model that used normal angle of incidence to oblique angle of incidence. The SALMON software we are using though cannot perform oblique angles of incidence due to development limitations and, so far, there are no planned updates in the near future to address our issue with the software. Due to this currently unsolvable issue, we were not able to perform any jobs in Hokusai.

3. Result

We discovered the limitation of the SALMON software, wherein it cannot be used to simulate models that use illumination set at an angle.

4. Conclusion

Now that we are equipped with the knowledge of SALMON's computational abilities and limitations, we will be able to fully utilize the available capabilities of SALMON for modelling other MIM plasmonic structures that are also designed for sensing various target gas molecules.

5. Schedule and prospect for the future

We are now designing another optical experimental system for gas sensing using normal laser illumination. We are currently in the process of determining the optimal experimental parameters such as new target gas molecule, laser wavelength, laser power, and nanostructure design. Once these experimental parameters have been set, we hope to once again have the opportunity to use Hokusai in FY2024 to simulate the electromagnetic properties of our nanostructure using SALMON.

6. If no job was executed, specify the reason.

No job was executed because we found out that the SALMON software we are using could not model electromagnetic waves at oblique angles of incidence. Unfortunately, based on our discussion with one of the creators of SALMON, this is a software development issue that is still a work in progress. Due to this issue, we could not move forward with our target simulations using SALMON and Hokusai.