Plasmonic refractive index sensor design

Finite-difference time-domain modeling and simulation for design and optimization of plasmonic nanohole array photodiodes

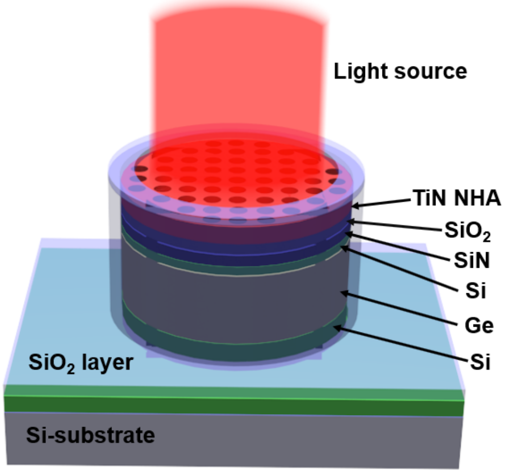

Figure 1: *Schematic sensor layout.*

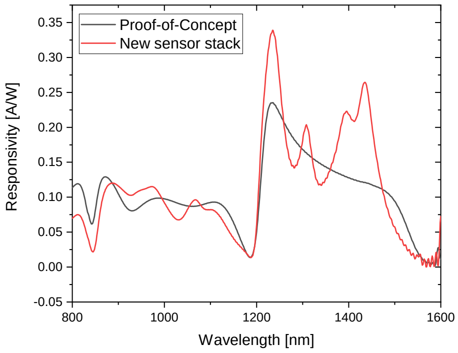

Figure 2: *Comparison of Proof-of-Concept[2] and new sensor stack.*

J. Schlipf, W. Han, S. Reiter, I. A. Fischer*, Chair of Experimental Physics and Functional Materials, BTU Cottbus - Senftenberg*

In Short

- Development of refractive index sensors based on plasmonic nanohole arrays and Germanium photodetectors
- On-chip integrated sensor with high sensitivity
- Investigation of different materials for plasmonic nanostructures and different optical sensor layer stacks
- FDTD simulation and multiscale optimization

For biological and medical applications, detection of biomarkers is becoming more and more important. The default methods rely on chemistry and spectroscopy, which require bulky and expensive instruments and are time-consuming. Nanobiosensors can solve these issues. Several pathways are being explored, including refractive index sensing via functionalized surfaces and surface plasmon resonance[1].

We have demonstrated collinear plasmonic nanohole refractive index sensor devices based on group IV semiconductor technology[2]. For possible future commercial applications, it is important to transform the concept from an academic lab environment to a commercial semiconductor foundry process. This is the main focus of our work together with project partners.

Fig. 1 shows the geometry of the proof-of-concept device. The plasmonic nanohole array (NHA) serves as spectral filter. Light is passed through via extraordinary optical transmission for selected wavelengths, depending on the refractive index of the superstrate. Since Si and SiO_2 are transparent in the wavelength range of interest between 1100 nm and 1600 nm, most of the light passing through the NHA is absorbed in the Ge photodiode below. The absorbed photons are converted into electron-hole pairs, which constitute the photocurrent.

The optical responsivity (Fig. 2) is defined as the ratio of photocurrent and light impinging on the device, and is the most important metric in the design. A change in superstrate refractive index will shift the responsivity spectrum along the wavelength axis, enabling detection. It is desirable to obtain a sharp responsivity peak with a steep slope. Various parameters have an influence on the responsivity peak. The height of the responsivity peak is determined by the thickness of the metal layer and the diameter of the hole as well as the thickness of the germanium layer. The peak position is determined by by the pitch of the NHA and the shape of the peak is determined by the layer thickness and the hole size.

To take into account requirements for layer thicknesses imposed by the fabrication process and enhance performance further, extensive nano-optical simulations are required. We employ a proprietary implementation of the finite-difference time-domain (FDTD) method[3] supplied by LUMERICAL[4] to solve Maxwell's equations.

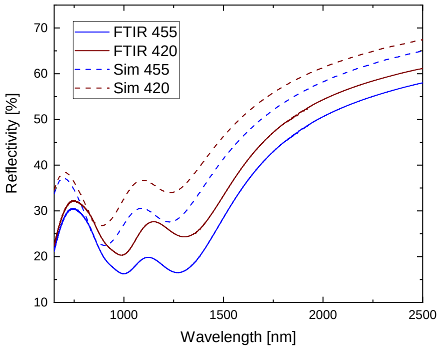

Figure 3: *Comparison of fourier-transform infrared (FTIR) reflectivity measurement results with FDTD simulation results for two nanohole array geometries.*

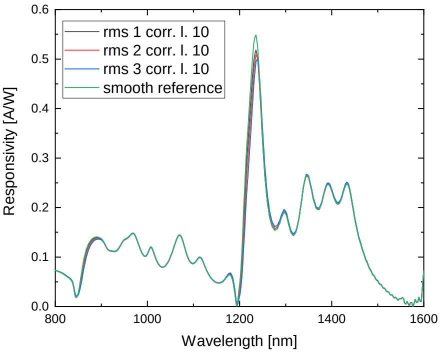

Figure 4: *Influence of rough Aluminium surfaces with a constant correlation length of 10 nm and different root mean square values of the surface roughness.*

FDTD employs two interlocking rectilinear grids for the electric and magnetic fields, periodically computing them from each other in time-domain. This eventually yields the impulse response of all grid points, which can then be converted to optical spectra via the Fourier transform. Our devices are periodic within the wafer plane, benefitting from the simplicity of periodic boundary conditions. FDTD is a mature and robust method, and parallelization is inherently possible by distributing parts of the simulation grid between computing nodes.

Previous FDTD simulations enabled us to significantly increase the calculated sensitivity compared to the proof-of-concept device[2] (Fig. 2). A further investigation of possible improvements is crucial for this project. We optimized a first batch of nanohole array geometries via FDTD, and reflectivity characterization results from fabricated devices are available (Fig. 3). Simulated and measured spectra show qualitative agreement. With our approach confirmed, we plan to refine our simulation further once a more detailed characterization of nanohole geometries and scattering losses in the measured reflectivity is available.

One particular focus is on the influence of sensor imperfections induced by the fabrication process. It is important to simulate these imperfections and their influence to the sensor behaviour. The most relevant imperfections are the surface roughness of the metal layer as well as the sidewall roughness of the nanoholes. These affect the propagation of surface plasmons, influencing the responsivity of the sensor. Aluminium (Al) and Titanium Nitride (TiN) NHAs are being investigated for different applications. For both materials it is necessary to investigate the influence of the roughness by simulation. To facilitate this, the accuracy of the simulation grid has to be improved, drastically increasing computational cost. Fig. 4 shows the simulated influence of different roughness parameters for an Al nanohole array on the optical responsivity.

In summary, an optical sensor is under development that reacts very sensitively to changes in the refractive index in the surroundings. For this purpose a plasmonic NHA is designed and the interaction of the NHA with various thin layers of the sensor stack are investigated. Predictions based on simulations are required in order to minimize the high prototyping costs in the course of development.

WWW

`https://www.b-tu.de/fg-exphysik-funktionale-materialien`

More Information

[1] A. Shakoor, J. Grant, M. Grande and D. Cumming, *Sensors* **19**, 7 (2019). `doi:10.1007/s10404-007-0198-8`

[2] L. Augel, Y. Kawaguchi, S. Bechler, R. Körner, J. Schulze, H. Uchida and I. A. Fischer, *ACS Phot.* **5**, 11 (2018). `doi:10.1021/acsphotonics.8b01067`

[3] K. Yee, *IEEE Trans. Ant. Prop.* **14**, 3 (1966). `doi:10.1109/TAP.1966.1138693`

[4] `https://www.lumerical.com/products/fdtd/`

Funding

This work has been funded by the Federal Ministry of Education and Research of Germany (BMBF) within the iCampus Cottbus project, grant number 16ES1128K.