Plasmonic refractive index sensor design

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

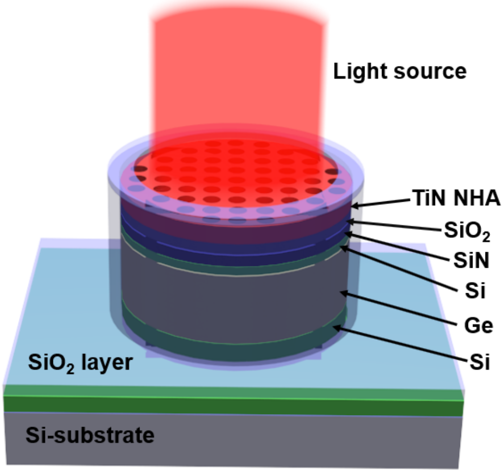

Figure 1: *Schematic sensor layout.*

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In Short

- Development of refractive index sensors based on plasmonic nanohole arrays and Germanium photodetectors
- On-chip integrated sensors 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 of rising importance. 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 resonances[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.

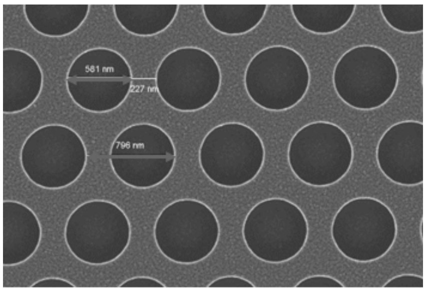

Figure 2: *TiN nanohole array fabricated at the Innovations for High Performance Microelectronics/Leibniz Institute for High Performance Microelectronics (IHP).*

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 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 influence the responsivity. 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 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 the deviations from design in geometry and material properties caused by the fabrication process and to further enhance sensing performance, 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.

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

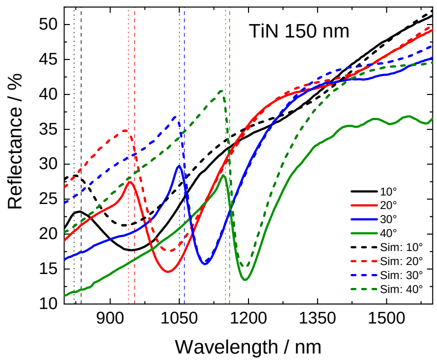

***Figure 3:** Measured and simulated reflectance spectra of NHA with different incident angles of p-polarized light.*

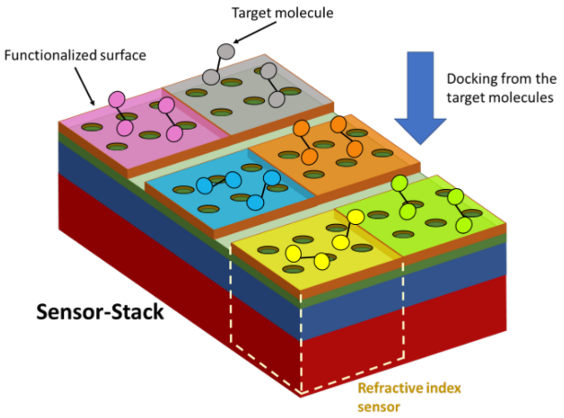

***Figure 4:** AgriNose project sensor concept. Shown is an array of various sensor segments with different functionalized surfaces. Each binds a spesific target molecule.*

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.

We used new measured spectra of fabricated nanohole arrays (Fig. 2) with different parameters and materials to fit our simulation parameters. This enables us to quickly and reliably determine the effects of design changes and adapt the behavior of the nanohole arrays to our requirements.

Due to the previous simulations, not only nanohole arrays but also the first prototypes of the complete sensor could be fabricated at the Leibniz Institute for High Performance Microelectronics (IHP). These prototypes are currently being experimentally characterized and then have to be further optimized. As soon as we have experimental data, our simulations will be adjusted. Then it is of great interest how the sensitivity of the sensor can be further increased. For this it will be necessary to simulate design changes in combination with different angles of incident light. For the new project AgriNose, additional simulations for a gradually varied refractive index on top of the sensors are required.

The AgriNose project is an adaptation for biosensing and is based on the prototype of the refractive index. The aim is to functionalize the sensor at the surface in such a way that gas molecules can selectively attach and be detected. The binding changes the refractive index at the surface, shifting the resonance of the NHA. The sensor is divided into several segments (Fig. 4), each responsible for detecting a different molecule. The composition of the detected molecules can, for example, be traced to diseases which have infected plants on a field. Simulations are needed to accurately design the sensor stack.

We have made great progress in increasing the performance of our NHAs. Further design improvements of the RI sensor have been made on base of our simulations and new prototypes were manufactured. The next steps are further optimizations of our NHA in the direction of alternative configurations of the holes and to optimize the performance regarding biosensing. In addition, the photocurrent measurement results of the RI sensor must be confirmed by means of simulations with regard to different surrounding dielectrics and angles of incidence.

WWW

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

More Information

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[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/

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