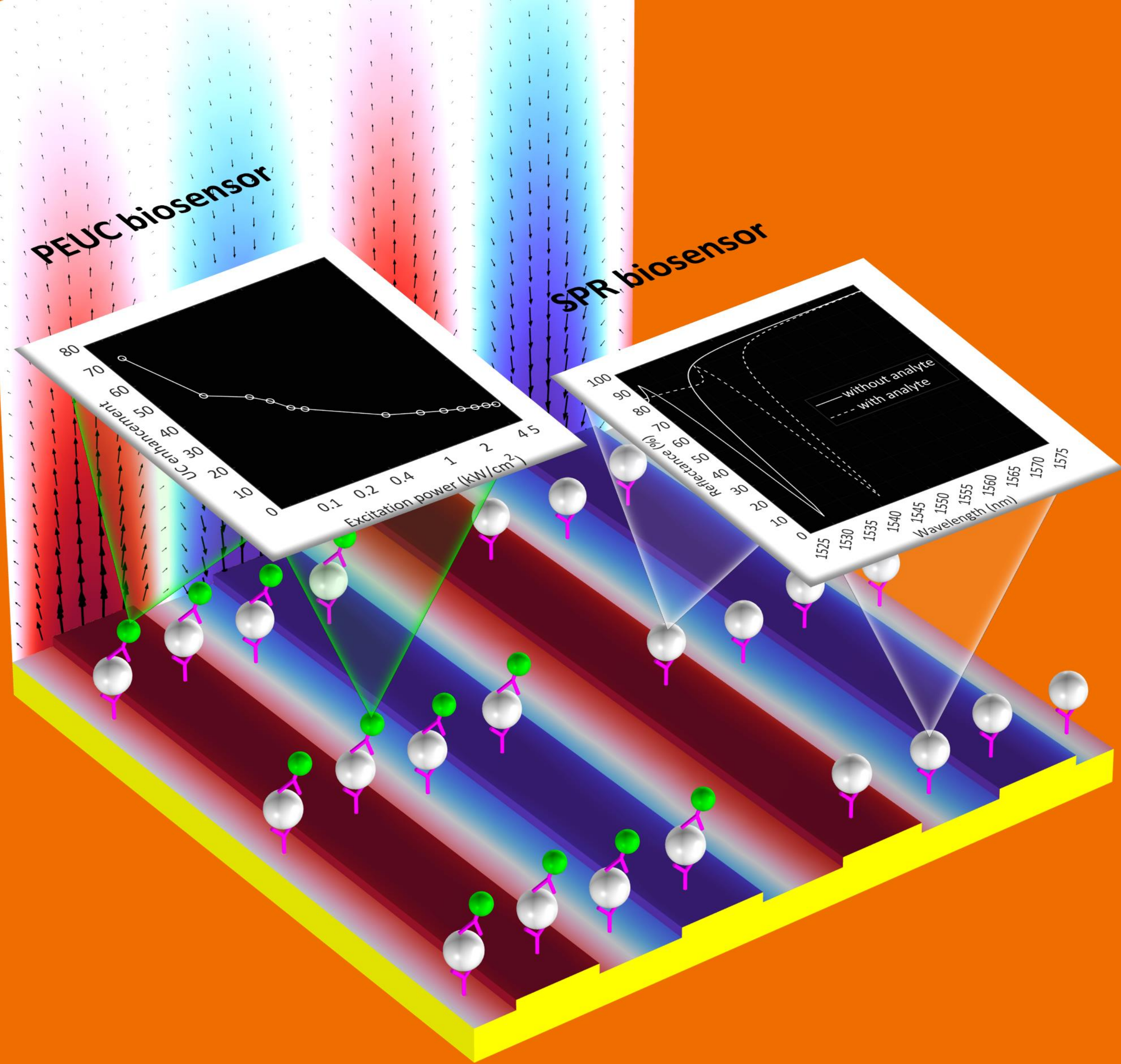


Numerical Simulation-Driven Design of Nanophotonic Biosensors

Computational modeling is needed for understanding, designing, and optimizing nanophotonic devices. Here, COMSOL Multiphysics® is employed for simulation-driven research and development of nanophotonic biosensors.

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Abstract

Nanophotonic biosensors are powerful analytical tools for quantifying biological molecules and particles with high sensitivity and specificity [1]. However, the fabrication of nanophotonic biosensors requires significant time and resources, which can make it a challenging and costly process. Therefore, computational modeling is crucial in comprehending the operational principles of such biosensors at a detailed level, but also in enabling effective design, optimization, and fabrication tolerance analysis of the

devices. This work demonstrates how COMSOL Multiphysics® efficiently designs, optimizes, and analyzes nanophotonic biosensors, thereby accelerating their development for diverse applications including diagnostics, biomedical research, and drug discovery.

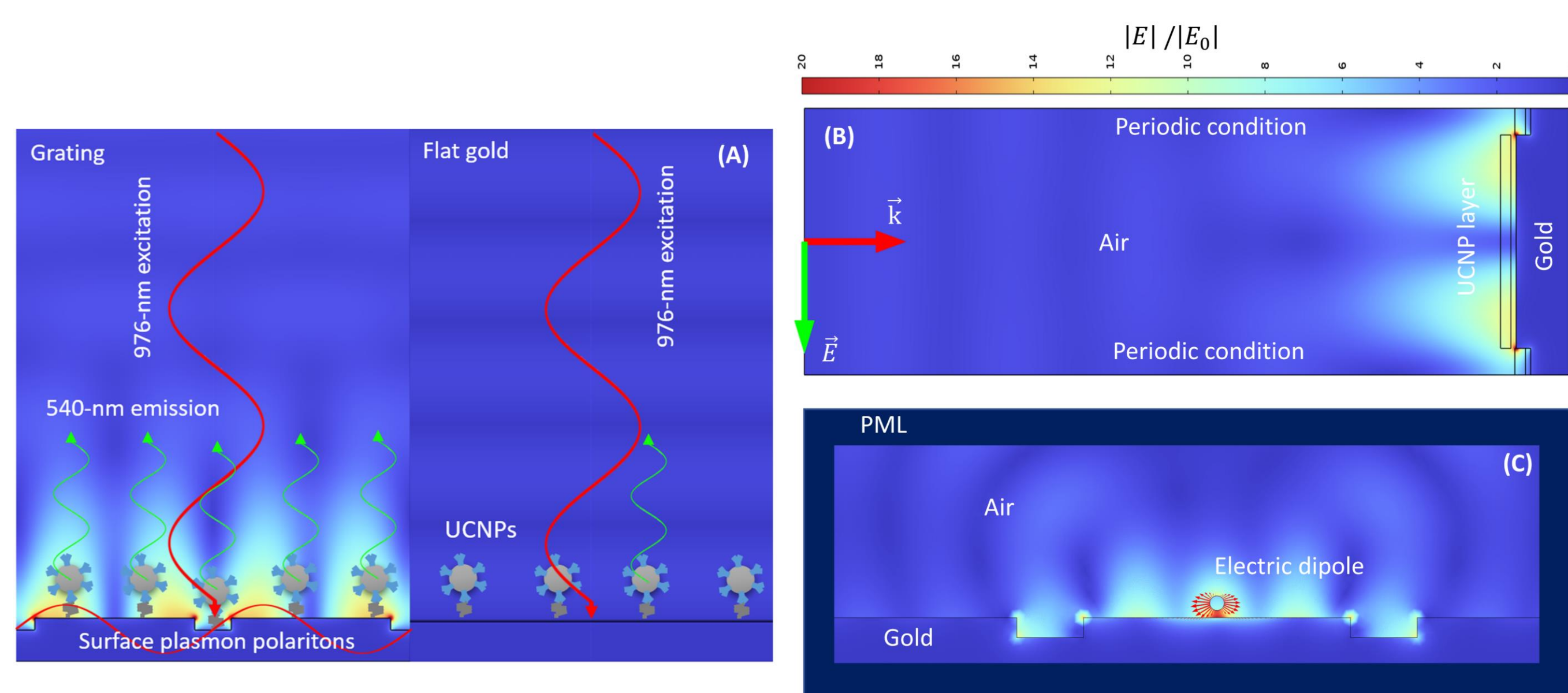


Figure 1. (A) Illustration of PEUC sensor. (B) Excitation model for optimizing SPP coupling at 976 nm. (C) Emission model for analyzing the quantum yield of a UCN at 540 nm.

Methodology

The Wave Optics Module is utilized to design, optimize, and analyze two different nanophotonic biosensors: plasmon-enhanced upconversion (PEUC) and surface plasmon resonance (SPR). In PEUC, enhanced upconversion signal improves the detection limit while the SPR wavelength depends on the analyte concentration on the surface.

In the PEUC biosensor (Fig. 1), a 976-nm excitation model and a 540-nm emission model are developed to optimize and analyze the enhancement of upconversion signal. The SPR sensor in Fig. 2 relies on grating-coupled surface plasmon polaritons (SPPs). The sensor is designed for a tunable laser working from 1528 nm to 1565 nm. The nanostructure of the sensor is optimized to maximize the sensitivity and the figure of merit, defined as the ratio between the sensitivity and the FWHM of the SPR dip.

Results

PEUC and SPR sensors are fabricated, characterized, and tested. Both sensors show a strong agreement between computational and experimental results.

The fabricated PEUC sensor achieves a hundred-fold enhancement in upconversion signal at low excitation power. The detailed results are discussed in our published paper [2]. This sensor is being applied to quantify cancer cell-derived exosomes.

The fabricated SPR sensor shows high sensitivity close to 1200 nm/RIU with a high figure of merit [3]. To our knowledge, such high sensitivity and figure of merit are previously unreported. The SPR sensor is used to sense glucose solution with a detection limit of 11 mM.

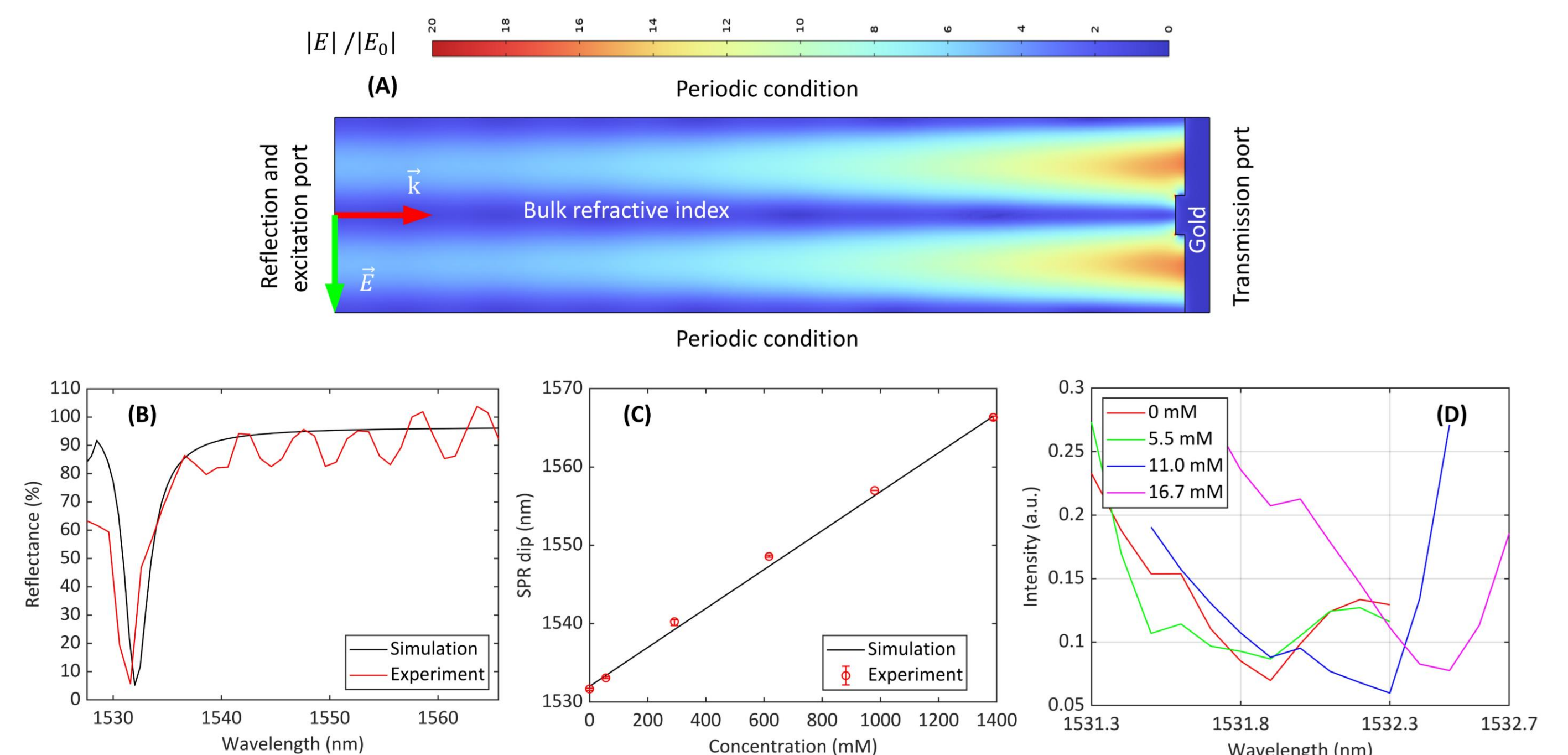


Figure 2. (A) SPR sensor model for bulk refractive index sensing. (B) Simulated and experimental reflectance spectra of SPR sensor. (C) SPR dip position as a function of glucose concentration. (D) SPR sensing at low glucose concentrations.

REFERENCES

- [1] J. Wang, S.A. Maier, and A. Tittl, "Trends in Nanophotonics-Enabled Optofluidic Biosensors," *Advanced Optical Materials*, vol. 10, no. 7, Apr. 2022.
- [2] D. Le et al., "Surface plasmon enhanced upconversion luminescence for biosensing applications," *Plasmonics in Biology and Medicine* XX, vol. 12396, no. 16, pp. 14–20, Mar. 2023.
- [3] D. Le et al., "High-sensitivity grating-based SPR sensor empowered by tunable laser", Markus Pessa International Summer School "New Frontiers in Optical Technologies", 7-11 August 2023, Tampere, Finland.

