Hochschule München University of Applied Sciences

Department of Applied Sciences and Mechatronics

HM Photonics Lab

Simulation of a temperature-compensated palladium-based fiber optic hydrogen sensor and comparison with measurements

Fabian Buchfellner[1]*, Qiang Bian[1,2], Alexander Roehrl[1], Fan Zhang[3], Wenbin Hu[3], Minghong Yang[3], Alexander W. Koch[2], Johannes Roths[1]

[1]Photonics Lab, Munich University of Applied Sciences, Munich 80335, Germany
[2]Institute for Measurement Systems and Sensor Technology, Technical University Munich, Munich 80333, Germany
[3]National Engineering Research Center for Optical Fiber Sensing Technology, Wuhan University of Technology, Wuhan 430070, China

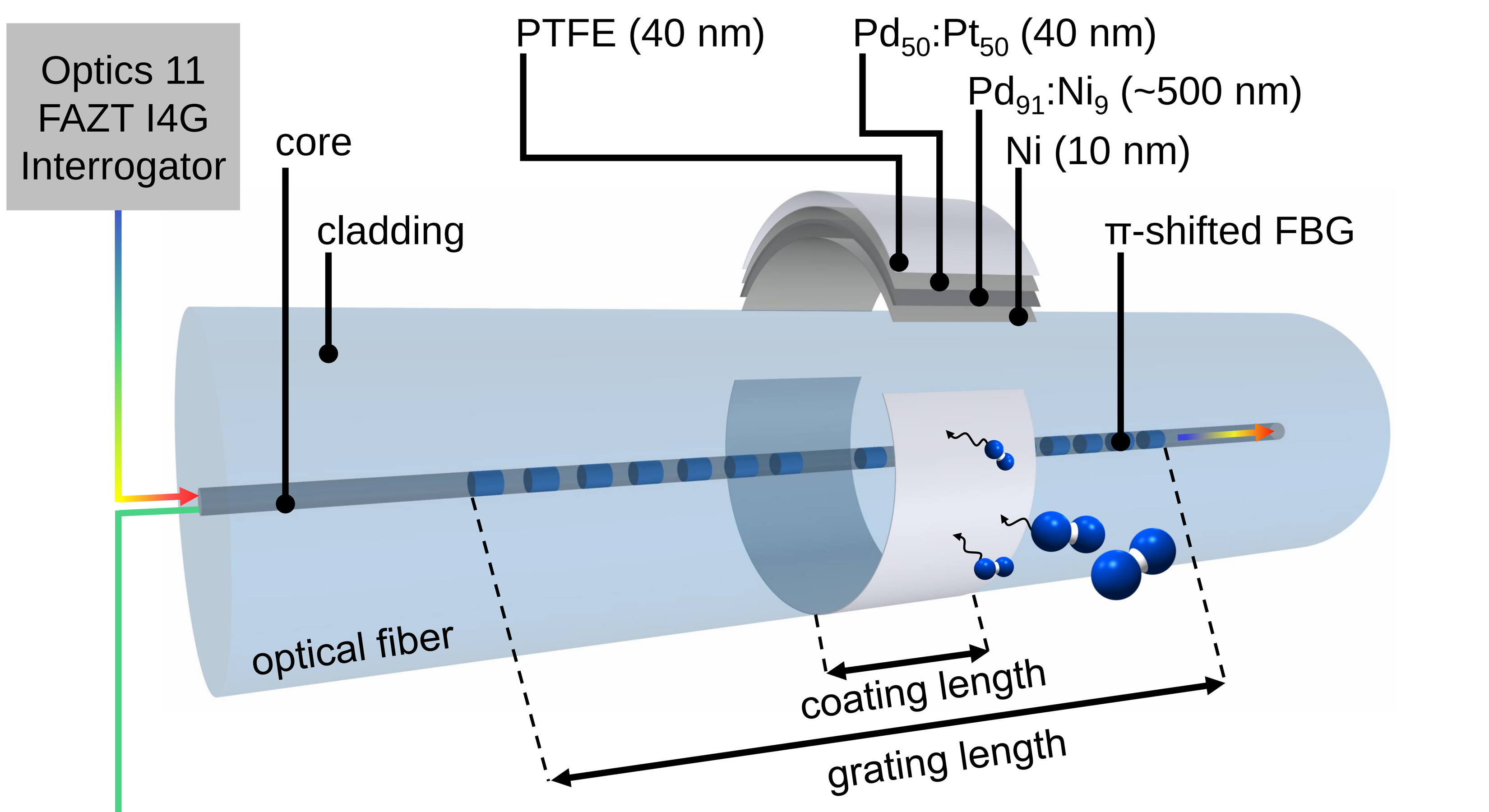
*fabian.buchfellner0@hm.edu; +49 89 1265 3654; http://fk06.hm.edu/pol/en/index.html

Abstract

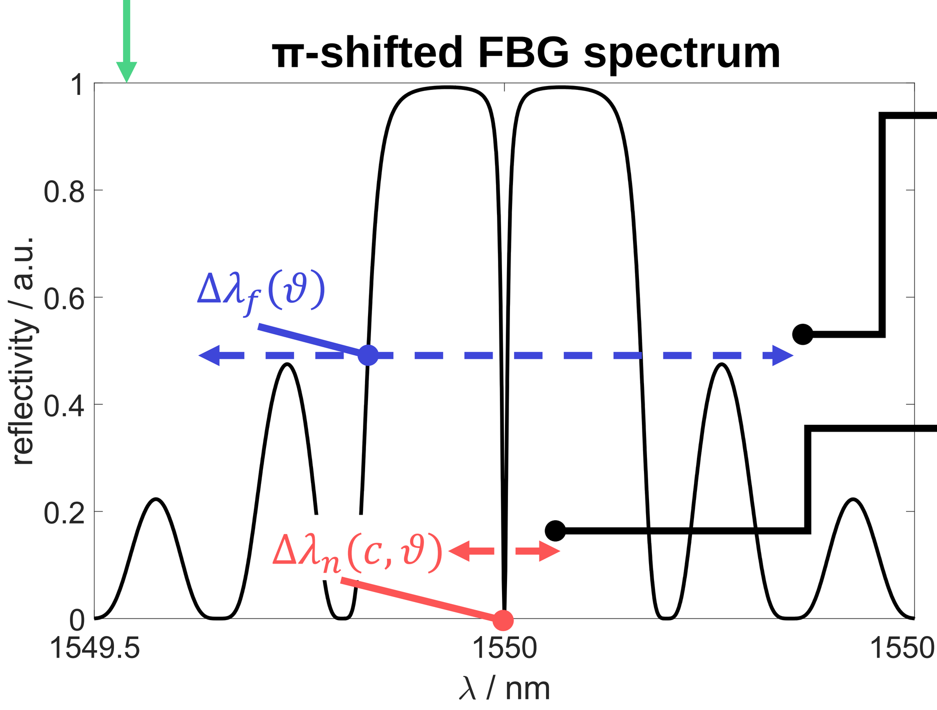
A temperature-compensated sensor architecture for a hydrogen sensor consisting of a partly palladium-coated pi-shifted FBG was modeled and compared with measurements. The transfer matrix formalism was used to compute the pi-shifted FBG with a hydrogen-induced, non-homogeneous strain distribution along the grating axis. The temperature response of the grating itself can be compensated by referencing the notch to the flank wavelength. In addition, the hydrogen solubility in Pd shows a non-linear temperature dependence that was also included in the sensor model. A comparison to measurements revealed good agreement with the simulation and highlights the potential of the proposed temperature-compensated hydrogen sensor.

Sensor principle and architecture

Palladium-based hydrogen sensing with FBGs:
Molecular hydrogen dissociates into atomic hydrogen that diffuses into the Palladium (Pd) bulk. This effect occurs at room temperature. Hydrogen occupies interstices in the Pd matrix and evokes an increase of the lattice constant, which macroscopically results in a volumetric expansion of the Pd. When FBGs are coated with Pd, the hydrogen-induced volumetric expansion leads to measurable strains within the FBG sensor. Pd alloys are used to improve response and durability of the nanofilms.



Simultaneous hydrogen and temperature measurement[1,2]:
To achieve multi-parameter sensing capability, a π-shifted FBG was utilized. Here, only a small section that contains the phase shift is covered with Pd. The wavelength that corresponds to the π phase shift – here notch wavelength - gets modulated due to hydrogen sorption.
When temperature affects the π-FBG, the entire spectral envelope will become subject to an equal wavelength shift, i.e., the notch and also the flank wavelength of the reflection spectrum will shift.



Envelope spectrum measured at the left flank $\Delta\lambda_f(\vartheta)$ goes with temperature ϑ

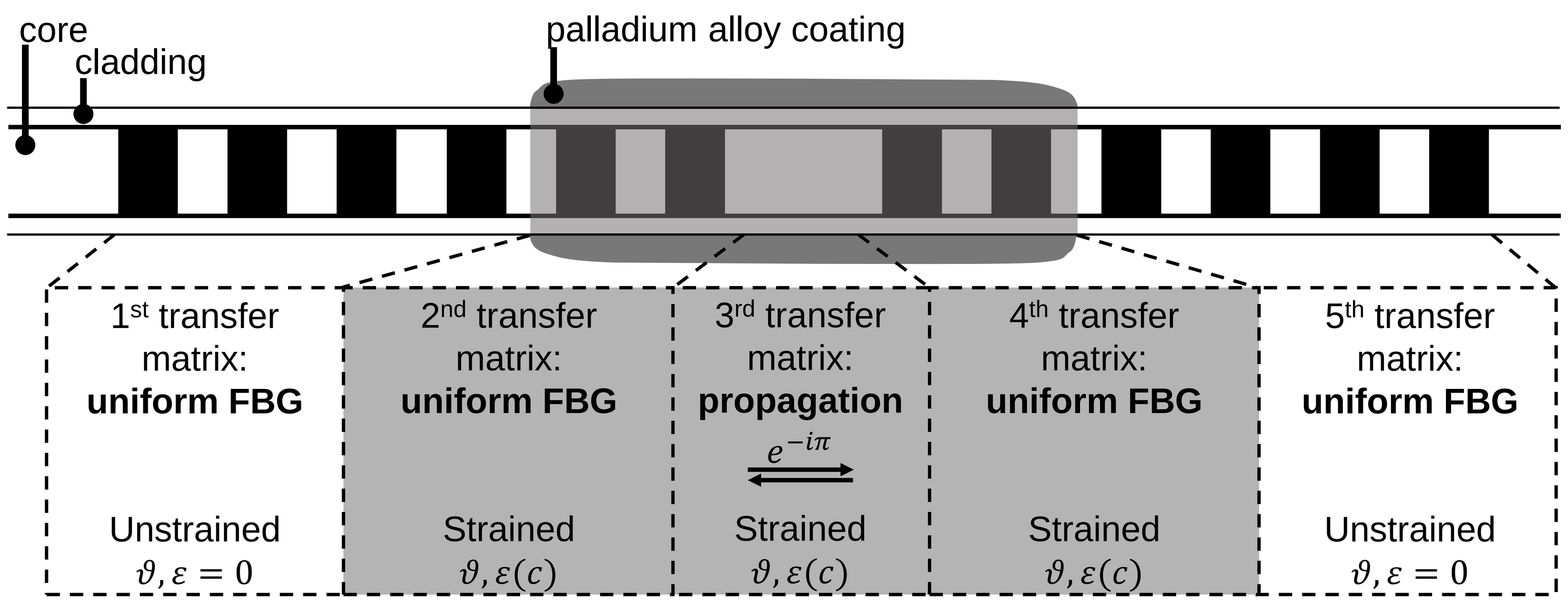
Notch wavelength $\Delta\lambda_n(c,\vartheta)$ goes with hydrogen concentration c and temperature ϑ

Temperature-decoupling due to referencing the notch to the flank:

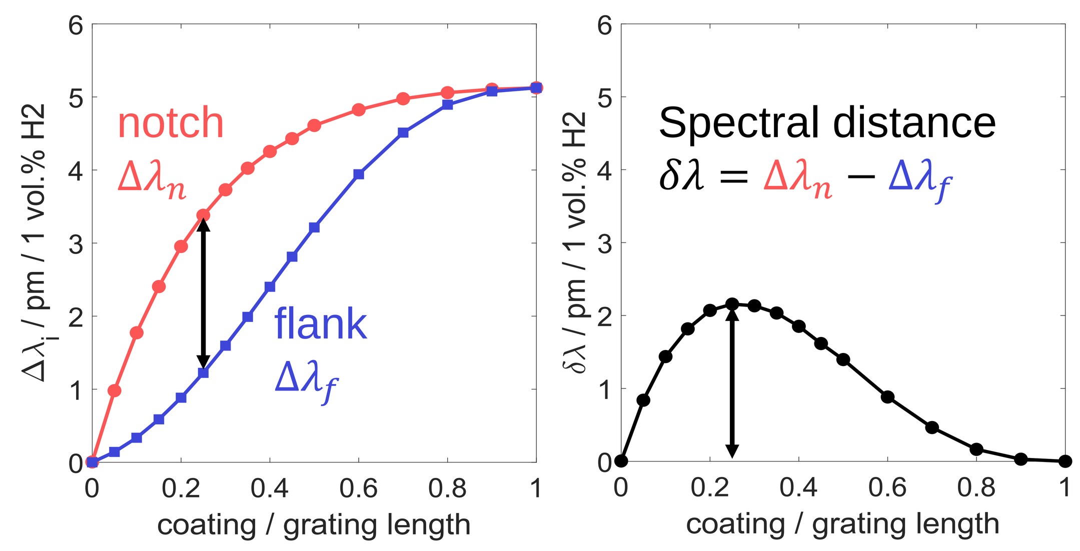
Spectral distance between notch and flank: $\delta\lambda(c) \equiv \Delta\lambda_n(c,\vartheta) - \Delta\lambda_f(\vartheta)$

Simulation approach and comparison with measurements

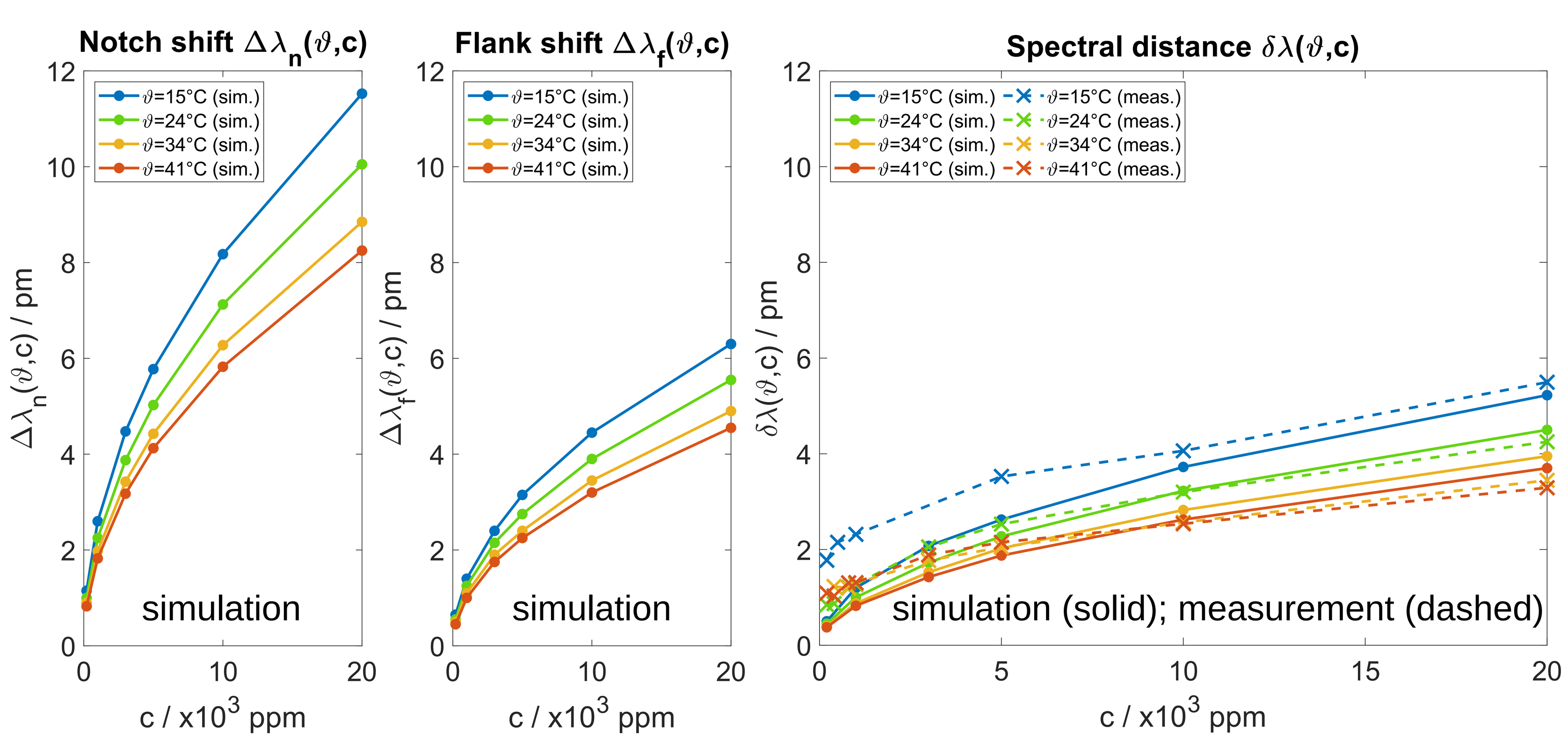
Simulation of the partly Pd-coated π-shifted FBG:
The reflection spectrum of a π-FBG can be computed with the transfer matrix formalism by stringing two uniform FBGs together with a phase delay of $\phi = \pi$ in between. For the spectrum of a partly Pd-coated π-FBG, where only a fraction of the full FBG is subject to H_2-induced strains, but all sections are subject to temperature, the model consists of two more uniform sections (shown below). Here, the outer two uniform sections do not experience H_2-induced strain ($\varepsilon = 0$) but temperature (ϑ). The inner two uniform sections and the propagation distance experience both temperature and strain. H_2-induced strains in Pd were computed with Sieverts' law for the temperature-dependent absorption of gases by metals.



Optimized coating-to-grating length ratio:
In reality, not only the notch but also the flank are subject to both H_2- and temp.-induced wavelength shifts. The optimum coating-to-grating length ratio obtained from simulations is 1/4.



Results and conclusion:
From Sieverts' theory it follows that the H_2 solubility depends non-linearly on temperature. Although the π-FBGs temperature response can be compensated by the sensor architecture shown above, the decreasing solubility in Pd with increasing temperature can be seen from both simulation and measurement:



For H_2 concentrations > 3000 ppm, the measurement agrees fairly well with the simulation (except at 15 °C). At concentrations < 3000 ppm, the data becomes diffuse, eventually induced by poor SNR and temperature instability during measurements. Nonetheless, the presented temperature-compensated hydrogen sensor architecture has high potential for real-field application, while further optimizations can be supported with the simulation work discussed above.

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1. Buchfellner, F., Bian, Q., Hu, W., Hu, X., Yang, M., Koch, A. W. and Roths, J., "Temperature-decoupled hydrogen sensing with Pi-shifted fiber Bragg gratings and a partial palladium coating," Opt. Lett., OL 48(1), 73 (2023)
2. Hu, X., Hu, W., Dai, J., Ye, H., Zhang, F., Yang, M., Buchfellner, F., Bian, Q., Hopf, B. and Roths, J., "Performance of Fiber-Optic Hydrogen Sensor Based on Locally Coated π -Shifted FBG," IEEE Sensors J. 22(24), 23982–23989 (2022).