

The power of using combinatorial materials science and finite element methods in the optimization of sensing by gold nanostructures

Peter Petrik^{1,2}, Deshabrato Mukherjee^{1,3}, Krisztián Kertész¹, Zsolt Zolnai¹, Zoltán Kovács¹, András Deák¹, András Pálincás¹, Zoltán Osváth¹, Dániel Olasz^{1,4}, Alekszej Romanenko^{1,5}, Thomas Siefke⁶, Sven Burger⁷, Miklós Fried^{1,8}, György Sáfrán¹

¹ Institute of Technical Physics and Materials Science, Centre for Energy Research, Hungarian Research Network, Konkoly Thege Miklós Str. 29-33, Budapest, 1121, Hungary,

² Department of Electrical Engineering, Institute of Physics, Faculty of Science and Technology, University of Debrecen, Bem tér 18, Debrecen, 4026, Hungary

³ Doctoral School of Materials Sciences and Technologies, Óbuda University, Népszínház u. 8, Budapest, 1081, Hungary

⁴ Department of Materials Physics, Eötvös Loránd University, Pázmány Péter Sétány 1/A, Budapest, 1117, Hungary

⁵ Doctoral School of Chemistry, Eötvös Loránd University, Pázmány Péter Sétány 1/A, Budapest, H-1117, Hungary

⁶ Friedrich-Schiller-Universität Jena, Albert-Einstein-Str. 15, D-07745 Jena, Germany

⁷ Zuse Institute Berlin (ZIB) & JCMwave GmbH, Takustraße 7, Berlin, 14195, Germany

⁸ Institute of Microelectronics and Technology, Kandó Kálmán Faculty of Electrical Engineering, Óbuda University, H-1084 Budapest, Hungary

petrik.peter@ek.hun-ren.hu

Summary:

Gold nanostructures were created using combinatorial magnetron sputtering and annealing, as well as by electron beam lithography to create nanostructures for plasmonic and Raman sensing. The optical response of the structures was measured by reflectometry, Raman spectroscopy and spectroscopic ellipsometry to study the accuracy of dimensional metrology and the performance of the structures for sensing. The structure was analyzed based on finite element calculations supported by electron microscopy measurements. The sensing performance of the deposited nanoparticles was explained by the density and size distribution on the surface as a function of the amount of deposited material. The measurements and finite element models on the grating structures revealed the most sensitive parameter ranges for dimensional metrology and sensing performance of the structures.

Keywords: Optical characterization, sensors, gold nanoparticles, plasmonics, combinatorial materials science, ellipsometry

Background, Motivation an Objective

The importance of plasmonic nanostructures in sensing doesn't need to be emphasized due to numerous studies and applications in recent years. The large number of possible configurations and combinations of materials necessitates powerful methods for the optimization and generation of databases of optical and structural properties. Combinatorial materials science is an established method with new optimized approaches [1,2] to improve the quality and controllability of the created materials and structures. The current work is a utilization of these opportunities for a range of materials properties for metrology and sensing.

Results

Two types of gold nanostructures have been investigated. The first one is created by annealing of gold layers with a gradually changing thickness on glass slides to generate gold nanoparticles for plasmonic and Raman investigations. The second type is a gold grating structure (Fig. 1) created by electron beam lithography. Both structures have been investigated by optical methods to determine the structures and to utilize them for (optical reflection and Raman) sensing. Finite element modeling and electron microscopy measurements supported the study by providing explanations of the sensing behavior of the structures. Both the gold nanoparticles created by sputtering and annealing and the grating structures created by electron beam lithography could be modeled using suitable finite element approaches. The simulations agreed

with measurements in both cases, explaining the major phenomena.

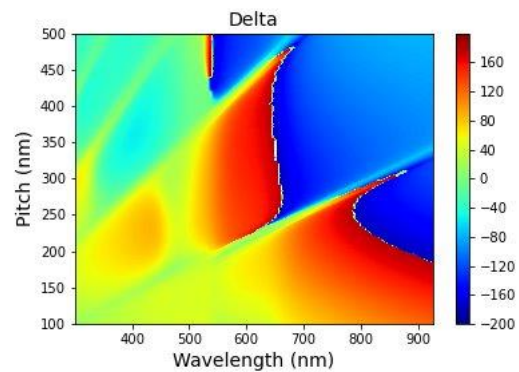


Fig. 1. Phase shift of the reflection coefficients of light polarized parallel and perpendicular to the plane of incidence as a function of the period (Pitch) and the wavelength on a gold grating in Kretschmann configuration ([glass ambient]/[gold grating (thickness of 60nm, grating line width of 50 nm)]/[water substrate]) at an angle of incidence of 70°.

References

- [1] G. Sáfrán, "One-sample concept" micro-combinatory for high throughput TEM of binary films, *Ultramicroscopy* 187 (2018) 50–55.
- [2] G. Sáfrán, P. Petrik, N. Szász, D. Olasz, N.Q. Chinh, M. Serényi, Review on High-Throughput Micro-Combinatorial Characterization of Binary and Ternary Layers towards Databases, *Materials* 16 (2023) 3005. <https://doi.org/10.3390/ma16083005>.
- [3] D. Mukherjee, K. Kertész, Z. Zolnai, Z. Kovács, A. Deák, A. Pálkás, Z. Osváth, D. Olasz, A. Romanenko, M. Fried, S. Burger, G. Sáfrán, P. Petrik, Optimized sensing on gold nanoparticles created by graded-layer magnetron sputtering and annealing, submitted for publication.