

Final Report of the project AKTION 92p16 (2022)

# AKTION project

## Glucose sensing using TiO<sub>2</sub> waveguides

Submitter, project coordinator: Dr. Valeria Butera, Central European Institute of Technology at Brno University of Technology (CEITEC BUT) – CZ

Project partner: Univ. Prof. Dr. Gottfried Strasser, TU Wien – AT

Additional participants: Ing. Stefania Isceri, Ing. Mauro David.

### **Activities of the Project during 2013 and 2014 during the period 1.1. 2022 - 31.12.2022.**

This project focused on intensifying the collaboration between the groups of Gottfried Strasser at TU Wien and Hermann Detz at CEITEC, Brno Univ. of Technology through staff exchange. Both groups share a common research focus related to the development and understanding of MIR spectroscopic devices. Specifically, within this project, CEITEC provided quantum chemical models for the adsorption of analyte molecules to the sensor surface, while TU Wien covered the design, fabrication and characterization of cascade laser-based MIR sensors.

### **Short description of the project activities.**

The scientific goal was to evaluate TiO<sub>2</sub> as a new MIR waveguide material, which is promising due to its biocompatibility.<sup>1</sup> The here proposed work extended a preliminary study by both groups, in which test devices, based on a grating coupler, a TiO<sub>2</sub> waveguide and a quantum cascade detector, were fabricated, and the adsorption mode and related adsorption energies of glucose on anatase had been calculated by cluster approach (CA) and periodic boundary condition (PBC) methods.

Within the project, TU Wien focused on the characterization of the TiO<sub>2</sub> based plasmonic waveguides for mid-infrared wavelengths, and the subsequent detection of the glucose using the TiO<sub>2</sub> waveguides coupled to a quantum cascade detector. On the other side, CEITEC performed a DFT study to understand the adsorption modes of glucose on TiO<sub>2</sub> surfaces.

### **The main activities of the staff (listed in alphabetic order of names):**

Dr. Valeria Butera visited TU Wien during the period 16.05.2022 – 20.05.2022. She got full access to the MIR optics labs at the Institute of Solid-State Electronics of TU Wien. During her stay, she was involved in the characterization of TiO<sub>2</sub> waveguides under the guidance of Mauro David. This research visit allowed her to get characterization skills of MIR optoelectronic devices and to perform the glucose detection experiments independently.

Ing. Stefania Isceri visited VB at CEITEC (12. – 13. 7.2022, 7. – 10. 11.2022, 12. – 14. 12.2022) to deepen her knowledge regarding DFT. She was involved in the modeling of higher d-glucose coverage on TiO<sub>2</sub> surface, and in the evaluation of the adsorption modes and adsorption energies. Stefania Isceri was provided with a VASP account and access to the IT4Innovation cluster for the duration of the project.

In addition, Stefania Isceri began work on a second topic, which may become a separate project in future. Thin films of thickness between 10 and 60 nm were grown on Ge(001) by MBE in the cleanroom facility of the Center for Micro and Nanostructures at TU Vienna. Then, they were transferred to the cleanroom facility of CEITEC (Brno), where they were characterized using scanning electron microscopy (SEM). The secondary electron (SE) imaging gave results about the surface morphology, putting in evidence diffuse flakes and small dots of different composition, whilst the mirror detector (MD) showed small dark spots attributed to holes or thinner regions.

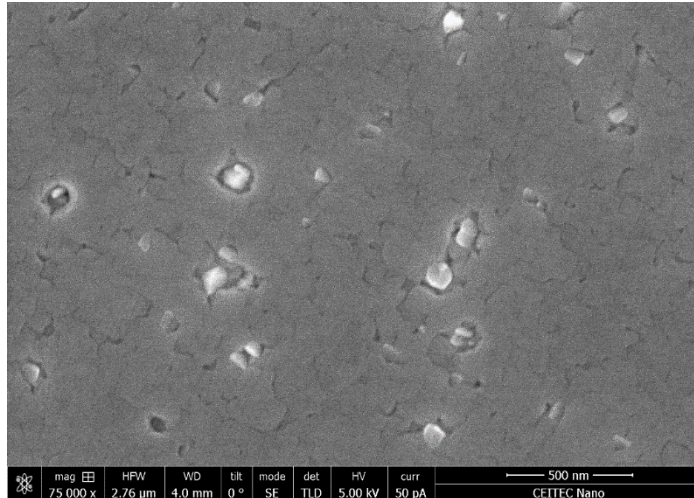


Figure 1 SEM image of the surface of YbRh<sub>2</sub>Si<sub>2</sub> on Ge(001) substrate

In addition, scanning transmission electron microscopy (STEM) specimens were prepared using focus ion beam (FIB) method. STEM is fundamental to complement the molecular beam epitaxy (MBE) study carried on at TU Vienna and to understand interface structural models for YbRh<sub>2</sub>Si<sub>2</sub>/Ge. Atomically resolved STEM images will be acquired and analyzed using the TITAN microscope in the cleanroom facility of CEITEC in the future.

### Impact

This project enabled and intensified the cooperation between CEITEC and TU Wien. The joint research work and visits provided the basis for a future joint proposal, e.g. within the CEEPUS or Horizon Europe schemes.

### Conference visits

The following conference presentations resulted from work that was carried out within the Aktion exchange project:

- S. Isceri, H. Detz, W. Schrenk, G. Strasser, M. Waas, R. Svagera, S. Bühler-Paschen, and A. M. Andrews, Single crystal growth of YbRh<sub>2</sub>Si<sub>2</sub>, DGKK-DEMBE, 16.05.2022 – 18.05.2022 Bremen, Germany, 2022, Presentation
- S. Isceri, M. Giparakis, E. Bakali, R. Svagera, M. Waas, D. Nguyen, H. Detz, W. Schrenk, S. Bühler-Paschen, G. Strasser, A.M. Andrews, "Strange metal YbRh<sub>2</sub>Si<sub>2</sub> grown by molecular beam epitaxy", North American Molecular Beam Epitaxy 2022, Oral Presentation, NM-TUM1-8, 18.09.2022 – 21.09.2022, Rehoboth Beach, DL, USA.
- S. Isceri, M. Giparakis, E. Bakali, R. Svagera, M. Waas, H. Nguyen, S. Paschen, H. Detz, W. Schrenk, G. Strasser, and A. M. Andrews, "Strange metal YbRh<sub>2</sub>Si<sub>2</sub> thin films ", Annual meeting of the Austrian physical society ÖPG 2022, 26.09.2022 – 30.09.2022, Leoben, Austria, 2022, Presentation

### References

- [1] B. Schwarz, P. Reininger, D. Ristanic, H. Detz, A.M. Andrews, W. Schrenk and G. Strasser, Nat. Commun. **5**, 4085 (2014).
- [2] V. Butera, A. Massaro, A.B. Munoz-Carcia, M. Pavone and H. Detz, Front. Chem. **9**, 716329 (2021).
- [3] V. Butera, H. Detz. Mater. Chem. Front., DOI: 10.1039/D1QM01118A.
- [4] A. Harrer, B. Schwarz, R. Gansch, P. Reininger, H. Detz, T. Zederbauer, A.M. Andrews, W. Schrenk and G. Strasser, Appl. Phys. Lett. **105**, 171112 (2014).