The physical phenomena behind the thermal reduction of TiO$_2$ surface

M. Rogala,$^a$ G. Bihlmayer,$^{b,c,d}$ P. Dabrowski,$^a$ C. Rodenbücher,$^e$ D. Wrana,$^f$ F. Krok,$^f$ Z. Klusek$^a$ and K. Szoł$^a$

$^a$ University of Lodz, Faculty of Physics and Applied Informatics, 90-236 Lodz, Poland

$^b$ Forschungszentrum Jülich GmbH, Institute of Advanced Simulation (IAS-1), 52425 Jülich, Germany

$^c$ Forschungszentrum Jülich GmbH, JARA - Fundamentals of Future Information Technologies, 52425 Jülich, Germany

$^d$ Forschungszentrum Jülich GmbH, Peter Grünberg Institute (PGI-1), 52425 Jülich, Germany

$^e$ Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research (IEK-3), 52425 Jülich, Germany

$^f$ Jagiellonian University, Marian Smoluchowski Institute of Physics, 30-348 Krakow, Poland

$^g$ University of Silesia, A. Chełkowski Institute of Physics, 40-007 Katowice, Poland

Titanium dioxide is a model material for the group of transition metal oxides, which makes it highly important for understanding the fundamental mechanisms of redox processes. The full description of physical phenomena in this material is required for further optimization of their applications. Especially TiO$_2$ is considered as memristive material in which resistive switching phenomena allow for information storage and can be utilized for the purpose of neuromorphic computing. We demonstrated the possibility of achieving a high density data storage in the surface layer of TiO$_2$ in our previous work [1]. This was related to the generation of quasi-homogenous switchable regions near the surface. Now we want to describe the origin of the formation of such crystallographic defects, responsible for the electronic properties of material. We will show that the thermal treatment in ultra-high vacuum conditions is only the initial step of the surface reduction making it electrically active. We will present that in fact other internal processes are responsible for the final properties of the surface layer relevant for its applications. With our X-ray photoelectron spectroscopy investigation supported by calculations we will elucidate the phenomena that determine the spatial distribution of the final stoichiometry of TiO$_2$, and decide about localization of defects structures responsible for electrical properties.

This work is supported by the National Science Centre, Poland (project 2016/21/D/ST3/00955) and by the German Science Foundation DFG (SFB 917 “Nanoswitches”).