Memoriu Activitate (Activity Report)

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My scientific career started roughly 7 years ago in the year 2019 right in the middle of the summer during the month of August. That's when i was employed by the Nartional Institute of Materials Physics (NIMP, Măgurele, România), in the Science of Surfaces and Interfaces laboratory, under the supervision of habil C.S. 1 Dr. Cristian-Mihail TEODORESCU. In these years, I co-authored 7 ISI articles, on which I am the first author at 3 of them. During these years at NIMP, I've participated on all the steps needed to create my career as a researcher: I've participated on most of the experiments handled in our laboratory, including the data measurements, analysis and data interpretation, all while looking for new ways to improve the management of time to data and optimize in the best way possible .I've also participated in the writings of most of the papers i co-authored. With all this in mind, I've been able to become self-sufficient when it comes to experiment managing and data analysis and I consider the next step in my scientific career as an independent researcher is to conduct my own project under the supervision of my Mentor.

The foundational training started when i was just admitted for my Master's Degree, when i was just learning what it means to focus only on surface techniques. I began by studying atomically clean semiconductors, specifically Ge (111), Ge (001) and Si (111) mastering the cleaning process using electron bombardment, often assisted by ion sputtering. I then began to study metal-semiconductor interfaces using the Molecular Beam Epitaxy (MBE) system. A significantly time-consuming but vital task was learning and perfecting the procedure of atomically clean any sample, which was always assisted by the Low Energy Electron Diffraction (LEED) technique to check the cristalinity and the degree of cleanness. I've also mastered deposition techniques of either thermal evaporation (TE) using resistive heating or by electron-beam evaporation (EBE). My Master's thesis consisted in the study of zirconium metal oxide layers deposited on Ge (001) for a preliminary study of hafnium zirconium oxide (HZO) using a laboratory X-Ray Photoelectron Spectroscopy (XPS). A paper was released based on the study of HfO2/GaAs (110) interfaces as a high-k dielectric material.

Beyond the experimental side, I have taken an active role in the structural maintenance of our laboratory's UHV systems. This included critical interventions such as replacing manipulator filaments, repairing evaporators that developed vacuum leaks, and participating in the complex process of opening and re-sealing the MBE and STM chambers. I was also responsible for the bake-out procedures and the calibration of evaporation rates using Quartz Crystal Microbalance (QCM), ensuring that the systems were always at peak performance for both internal research and external collaborations.

During my PhD studies, I've already become fully self-sufficient when it comes to managing experiments, my focus shifted towards studying ferroelectric materials. Initially, I tried synthesizing ferroelectric HfO_2 layers in order to make high-quality HZO heterostructures, but obtaining the orthorombic phase proved to be too difficult with our current setup. That's when I started using ferroelectric barium titanate ($BaTiO_3$, BTO) deposited on nobium-doped (0.5% Nb) strontium titanate (STON). This sample was made in collaboration with another laboratory within the same institue using a pulsed laser deposition technique (PLD). From this point forward, the core of my experiments was conducted at the Elettra Synchrotron in Trieste, Italy.

My first major doctoral study focused on the adsorbtion and desorbtion of carbon monoxide (CO) on ferroelectric barium titanate. The underlying mechanism relied on the ferroelectric properties: when the surface loses its polarization, the molecular gas desorbs. A few main things were needed to be checked in this study: i) derrive the composition of BTO at each stage; ii) derrive the BTO termination, iii) derrive the polarization orientation, iv) verify the stability of the sample, v) derivation of the amount of CO adsorbed and the state in which it's adsorbed. For this, the BTO sample needed to be atomically cleaned by electron bombardment heating in a rich O_2 atmosphere at rougly 850 °C. The surface was verified with XPS and upon measurements a residual carbon contamination of roughly 5% remained on the surface, an amount which couldn't be removed no matter how much heating was applied. The CO dose was similar in all cases, 5 × 10–6 hPa for 15 mins, aprox. 3.4 kL. We found out that CO is adsorbed in a non-dissociated way thanks to its considerably low polarization (about 0.2-0.3 C·m–2). In the end we were able to find an answer for each of our question. The most important one is its stability, where the BTO composition remains mostly unchanged thorough the whole experiment. Thanks to the synchrotron radiation, we identified the surface to have a termination in BaO and from the band-bending effects an outwards polarization was deduced. Finally the amount of CO adsorbed ranges from one molecule for ten surface unit cells with an increase of 30% for adsorbtion below room temperature [Iancu et al. Mater. Adv., 5, 5709 (2024)].

The second major study consists on the adsorbtion and desorbtion of ethylene on BaO-terminated (001) barium titanate surface, where carbon is detected in an oxidized state, with binding energies similar to those resulting from the adsorbtion of CO on $BaTiO_3$. The amount of carbon adsorbed on the surface is also similar to the case of carbon monoxide and upon heating the sample, the polarization is lost and the oxidized carbon signal vanishes. The most important aspect was that there was no noticeable oxygen loss upon the repeated cycles of adsorbtion/desorbtion [Iancu et al. Heliyon, 10, e35072 (2024)]. My last major work also concluded my PhD research by studying the adsorption of molecular CO_2 on $BaTiO_3$ with it being a record earning article for how fast was completed from the time experiments were finished to the day the article was accepted, which took just under 3 months for this whole procedure. The amount of CO_2 adsorbed is derived to be between one molecule for a surface BaO unit cell (adsorption below room temperature) and one molecule for two unit cells (adsorption above room temperature). The molecule is bound with its carbon to surface oxygen, forming a CO_3 structure. The $BaTiO_3$ (001) surface is unaffected by the repeated cycles of adsorption-desorption [Iancu et al. Mater. Adv., 5, 8798 (2024)]. All these studies enabled me to finish the PhD thesis with the title „Controlul Feroelectric al Adsorbțiilor și Desorbțiilor Moleculare pe Suprafețe Monocristaline (001) de Titanat de Bariu" all thanks to my coordinator Cristian-Mihail TEODORESCU.

My expertise in X-ray Photoelectron Spectroscopy has also been utilized in collaborative efforts with other research entities, such as Emil Pavelescu from IMT Bucharest. I managed the characterization of over 30 external samples, providing not just the raw measurements but also complex data deconvolution and chemical state identification. This activity allowed me to encounter a vast array of materials beyond my primary research focus, further deepening my understanding of surface chemistry and electronic properties. This vast majority of data from either internal or external experiments allowed me to also take part in the national research infrastructure thanks to my contributions to the IOSIN and Nucleu projects by offering to write multiple reports about our experiments at NIMP and offering help to my colleagues in need when they were struggling with deadlines facing them.

Having achieved scientific self-sufficiency through my doctoral studies, I consider the next natural step in my career to be transitioning into an independent researcher capable of conducting my own projects. Moving forward, I propose to build upon my expertise in ferroelectric surfaces and ultra-high vacuum techniques to develop new methodologies for capturing greenhouse gases and volatile organic compounds. Furthermore, I plan to continue extending our laboratory's international reach by writing new proposals for beamtime at major synchrotron facilities. I will also remain actively involved in the LIMSAE laboratory framework, ensuring the continuous training of new colleagues and the maintenance of our complex multi-method systems.