Final Report

Project acronym: SIOX
Project number: 4288
M-ERA.NET Call 2016

Period covered: 01/06/2017 to 31/05/2020

Coordinator:

Dr. Matjaž Spreitzer
matjaz.spreitzer@ijs.si
Jožef Stefan Institute , Jamova 39, 1000 Ljubljana, Slovenia

Publishable project summary

Project *SIOX (*Engineering of silicon-oxide interface using the pulsed laser deposition technique) exploited rich functionalities of oxides and their heterostructures with great promises within the emerging field of oxide electronics. For their implementation, epitaxial integration of oxides with silicon (Si) platforms using industrially appropriate technology is urgently needed, and its development represented the main goal of SIOX. However, such integration is extremely delicate due to materials' intrinsic incompatibility. This challenge was addressed by a collaboration between three research groups, from the Jožef Stefan Institute (JSI), the University of Liege (ULg) in Belgium and the University of Twente (UT) in the Netherlands, with expertise in the field of atomically controlled growth, theoretical modeling, and materials' applications.

Pulsed laser deposition (PLD) was used for the growth of different oxide heterostructures, which were then analyzed by several complementary techniques including: reflection high-energy electron diffraction (RHEED), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), scanning tunneling microscopy (STM), atomic force microscopy (AFM) and transmission electron microscopy (TEM) as well as a number of functional characterization techniques. Experimental studies were supported by computational modelling based on Density-functional theory (DFT).

We used DFT calculations to study the growth of thin films of functional oxides on Si. Various theoretical structures of Sr-terminated Si surfaces and $SrTiO_3$ (STO)-Si interfaces were modelled. It was found that one complete atomic layer of Sr is needed for the formation of a STO-Si interface with open Si dimers. Additionally, atomic models of Sr-buffered Si surfaces were used to explain the origin of surface defects observed in high-resolution STM images of PLD-grown Sr/Si surfaces. These STM images represent the first local structural analysis of such surfaces at an atomic scale and demonstrate that PLD can be applied to grow high-quality Sr-buffered Si surfaces. As-prepared surfaces were then used for the epitaxy of STO thin films on Si. A detailed analysis of the initial deposition parameters proved to be extremely important, as the parameter window for successful growth is very narrow. All the gained knowledge led to a development of a protocol for a complete control of silicon-oxide interfacial reactions and overgrowth of a single-crystalline STO thin films with optimized buffer and template stoichiometry, which is the main achievement of the project. In the last part of the project, multiple approaches for integrating oxide heterostructures on Si were used, including the STO-Si pseudo substrates. Various functional oxide films, heterostructures and supperlattices were prepared using PLD. The typical layer-by-layer growth mode and atomically flat surfaces were achieved for all films, comparable with the films on single-crystal STO substrates. In the case of $LaMnO_3$/STO supperlattices, the highest crystallinity of the film was observed on STO-coated $Ca_2Nb_3O_{10}$ (CNO) nanosheets, owing to the small lattice mismatch between CNO and STO as well as less clamping from the Si substrate.

Both main objectives of the project were accomplished. We developed a procedure for the preparation of high-quality oxides on Si, based on gained knowledge and understanding of the corresponding interface phenomena, and we demonstrated functionalization of as-prepared layers. These results will facilitate the exploitation of the rich electrical, magnetic, and optical properties of oxides and their heterostructures for the development of next generation electronics.