Project No.1.1.1.1/18/A/073

Duration of the project: 01.03.2019. – 28.02.2022.

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Project Implementers: The Institute of Solid State Physics, University of Latvia (ISSP UL) in collaboration with the vacuum coating SME company Sidrabe Vacuum Ltd.

On the implementation of the project (period 01.11.2019. - 31.01.2020.)

Among the most important achievements in Latvian science 2019 are also researchers of the Project No 1.1.1.1/18/A/073: Dr. Roberts Eglītis, Dr.Juris Purāns.

As part of Project No 1.1.1.1/18/A/073 "Smart Metal Oxide Nanocoatings and HIPIMS Technology" metal oxide coating samples were made. In the framework of the project activity "Development of the application technology for reactive R-HiPIMS TMO thin film application" injection gas and optical emission systems were adjusted to obtain necessary process parameters and the planned studies were carried out.

Testing results for injectable gases and optical emissions systems were analysed and conclusions were re ached. The planned sample coatings were manufactured, described and the data for the parameters of the coating technological process was prepared. The coverage process parameters were optimized accordin g to the results of the coating measurement analysis.

Research on the synthesis of ReO3 thin films has been continued in the framework of the project activity "Production of the TMO samples and optimization of the reactive R-HIPIMS parameters". Successfully developed ReO3-WO3 thin films deposition technology using magnetron sputtering and thermal anneling methods. The ten ReO3-WO3 thin films samples were selected and characterized. Preparation, description of the sample coatings and data of the parameters of the technological process of coating were prepared and presented. The parameters of the coating process were re-optimized according to the results of the coating measurement analysis.

During the reporting period, the technical report on the design of the R-HiPIMS power supply in a chamber with two magnetic elements was supplemented. Injection gas and optical emission systems were adjusted to obtain optimum process parameters. The planned metal oxide coatings were manufactured. The effect of technological coating process parameters on the reactive HiPIMS coating results was analyzed.

Preparation, description of the sample coatings and data of the parameters of the technological process of coating were prepared and presented. The parameters of the coating process were re-optimized according to the results of the coating measurement analysis.

We performed B3LYP and B3PW calculations for the upper three layer atom relaxation for the BO2-terminated $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$ as well as ReO_3 (001) surfaces. It is worth to notice that the ReO_3 has exactly the cubic ABO_3 perovskite structure, but with the only exception, missing A atom. For the case of $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$ perovskites as well as ReO_3 BO_2-terminated (001) surfaces, according to our calculations, all upper layer atoms relax in the direction towards the bulk. The ReO_2-terminated ReO_3 (001) surface upper layer Re atom displacement magnitude (3.19% of a_0) is larger than the calculated ABO_3 perovskite BO_2-terminated (001) surface B atom relaxation magnitudes, which are in the range from 1.30% of a0 for the $CaZrO_3$ till 2.37% of a0 for the $PbZrO_3$. Just opposite, all $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$ perovskite second layer atoms relax outwards. The only exception from this systematic trend is the second layer ReO_2-terminated ReO_3 (001) surface O atom inwards relaxation in the direction towards the bulk by a very small relaxation magnitude of -0.32% of a_0. All third layer atoms for BO_2-terminated $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$ as well as ReO_3 (001) surfaces, again, relax inwards, towards the bulk. Nevertheless, the relaxation magnitudes of all first layer atoms for $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$ as well as ReO_3 BO_2-terminated (001) surfaces are much larger than the relaxation magnitudes of the third layer atoms.

In the framework of the project activity “Characterization of the obtained TMO and EC samples”, structural and morphology analysis were performed (XRD and SEM measurements), as well as optical (light absorption and transmittance in UV-VIS region) and electrical properties (electrical conductivity and charge carrier mobility) were studied of the as-prepared thin films in relation to the synthesis parameters. EXAFS measurements were also performed on amorphous ReO_x-WO_{3-x} and crystalline ReO_3, WO_3 thin films.