Applied Surface Science
Room 116 - Session AS-MoA

Chemical Processes at Surfaces

Moderators: Jordan Lerach, PPG Industries, **Alexander Shard**, National Physical Laboratory

1:30pm **AS-MoA-1 Investigating the Chemical and Physical Changes of the Boehmite Layer as a Result of AA6061 Surface Etching and Film Growth Time***, **Lyndi Strange**, S. Niverty, M. Bowden, S. Tripathi, R. Shimskey, J. Wierscheke, M. Pole, V. Joshi,* PNNL

Low-enriched uranium alloyed with 10% Mo (U-10Mo) is currently being considered to replace high-enriched uranium in research reactors. The configuration consists of a U-10 Mo plate fuel with a 25 µm Zr interlayer barrier with an AA6061 alloy. The AA6061 alloy can be coated with boehmite (an aluminum oxyhydroxide) to prevent corrosion due to its high pH passivation range. Boehmite coatings are usually formed on AA6061 substrates via autoclave processing in alkaline media. Before boehmiting, the AA6061 can be cleaned via dry polishing or wet etching, which can cause changes in the surface likely affecting boehmite nucleation sites and subsequent adhesion to the AA6061 substrate. In this work, we seek to understand how the AA6061 pre-treatment methods as well as the boehmite layer thickness affect the chemical composition of the layer, corrosion resistivity, and adhesion to the AA6061 substrate. X-ray photoelectron spectroscopy (XPS) was used to determine the surface chemistry of boehmited samples as well as etched AA6061 samples. Grazing incidence X-ray diffraction (GI-XRD) was used to investigate aluminum oxide derivatives throughout the boehmite layer. For a more in depth investigation of aluminum oxide derivatives, transmission electron microscopy (TEM) was used to examine the differences at the interface of the AA6061 and boehmite. Tribology analysis was used to gain insight to boehmite adhesion onto the AA6061 substrate and changes as a result of pre-treatment. Lastly, the corrosion resistivity was examined using electrochemical techniques such as potentiodyanamic polarization (PD), electrochemical impedance spectroscopy (EIS), and long-term corrosion experiments which gave insight to the oxidation dynamics of the coating and oxide layer resistiveness. techniques allow a clear delineation of how the different etching techniques and layer thickness affect the overall physical properties of the formed boehmite layer as well as explain variation in the interfacial properties of the AA6061/boehmite. These results provide insight to the most efficient and highest quality method to grow boehmite on the surface of AA6061 for use in research reactors.

1:45pm **AS-MoA-2 SiO_2 Surfaces Sputtering Profiles: Experimental and Numerical Study***, **Camil Bocaniciu**, J. Pichler, A. Celebi,* TU Wien, Austria*; M. Ostermann,* CEST GmbH, Austria*; M. Valtiner,* TU Wien, Austria

Silicon dioxide (SiO_2) crystals serve as a relevant material in sputtering processes for their well-defined properties and broad applications in material science. The material offers a stable, reproducible target, aiding in the accurate calibration of sputtering equipment and standardizing experimental conditions. This stability is crucial for developing thin films, coatings, and semiconductor devices, where precise material control is essential [1].

The objective of this study is to explore the atomic layer structure and the composition of SiO_2 surfaces at different thicknesses from both experimental and numerical point of views. We first measure depth profiles of different thicknesses of SiO_2 using Low Energy Ion Spectroscopy (LEIS) at various energies. LEIS is a highly surface sensitive technique which probes only the top atomic layer of a material surface [2]. Our findings indicate that combining sputtering with LEIS is an effective technique for probing the in-depth structure of SiO_2 crystals grown on Si substrates. Distinct profile variations were observed for different surface oxidation processes, including O_2 plasma, thermal oxide, and native oxide, particularly for oxide thicknesses varying between 1.2 to 2 nm. In contrast, for thicker oxides between 30 and 60 nm, the profiles converged, showing minimal dependence on the oxidation method employed.

To provide additional physical insights into the obtained depth profiles by LEIS measurements, we subsequently perform sputtering simulations using SDTrimSP [3]. Sputtering simulations calculate the interaction between incident ions and surface atoms and describe sputtering, as well as surface degradation and ion implantation in the target material. For Ar^+, simulations demonstrate preferential sputtering of oxygen compared to silicon and suggest a layer intermixing in SiO_2 of 1.2 nm for 0.5 keV incident ion energy and 3.2 nm for 2 keV incident ion energy. Our simulations further show that simulated sputtering depth profiles correlate well with the depth profiles obtained by the LEIS measurements. Ultimately, the well-established stoichiometry of SiO_2 will be used as a reference for oxygen content by integrating experimental measurements with simulation results. This method will enable quantification with LEIS for any material surface that contains oxygen

[1]Kelly, J. J. (2003) "SiO2: A Versatile Reference Material for Sputtering and Thin Film Research." Journal of Vacuum Science & Technology A, vol. 21, no. 4.

[2]Brongersma, H. H., Draxler, M. (2007). Surface composition analysis by low-energy ion scattering. Surface Science Reports, 62(3), 63-109.

[3]Mutzke, A. et al. (2019) “SDTrimSP Version 6.00”

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