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In situ X-ray photoelectron spectroscopy study of atomic layer deposited ceria on SiO_2: substrate influence on the reaction mechanism during the early stages of growth — •Max Gertig, Carlos Morales, Karsten Henkel, and Jan Ingo Flege — Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology Cottbus-Senftenberg, Konrad-Zuse-Straße 1, 03046 Cottbus, Germany

Atomic layer deposition (ALD) is known to produce amorphous and defect-rich films in a layer-by-layer fashion, which can potentially give rise to unexpected material properties. In particular, ultrathin films (few monolayers) will show the highest complexity, as the substrate-material interaction will play a major role during deposition. Therefore, it is crucial to understand the early stages of growth of the ALD process to control and potentially tailor this interfacial interaction. Applying a surface science approach combined with complementary ex-situ characterization, we have studied by in-situ X-ray photoelectron spectroscopy (XPS) the early stages of ceria (CeO_x) growth on SiO_2 substrates deposited by thermal-ALD using $Ce(thd)_4/O_3$. Interestingly, an initial mixture of Ce^{3+} and Ce^{4+} was observed, although only Ce^{4+} may be expected considering the used precursor and oxidant. This fact, together with a deviation from the ideal layer-by-layer growth and a higher growth rate during the first cycles, indicates a significant influence of the substrate of the ALD reaction mechanism as well as a correlation between morphology and ceria oxidation state.

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