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Growth and Structure of Epitaxial Ce1-xZrx02 Thin Films on Yttria-Stabilized Zirconia(111)

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We describe here studies aimed at the identification of optimum parameters for the epitaxial growth of the mixed-oxides films, $Ce_{1-x}Zr_xO_2$ with x = 0.1, 0.2 and 0.3, by oxygen-plasma-assisted MBE on single crystal Y-stabilized ZrO_2 (YSZ) substrates. The resulting films were characterized by RHEED, LEED, XPS/XPD, RBS/C in order to determine their bulk and surface structures and compositions. Pure-phase, epitaxial $Ce_{1-x}Zr_xO_2$ films readily grew on YSZ(111) without showing any contamination of yttria from the substrate. The resulting epitaxial film surfaces are unreconstructed and exhibit the structure of bulk CeO_2(111). XPS data indicate that both Ce and Zr cations are formally in the +4 oxidation state for all films prepared here. Small differences in the photoemission results for Zr-doped ceria films as compared to those obtained for pure ZrO_2 may be explained by changes in electronic structure when Zr is added to ceria that, in turn, results from longer Zr-O bond distances in the mixed oxides. The minimum yields obtained from the random and channeling spectra of these films also provide evidence that high quality single crystal CeO_2 and $Ce_{0.7}Zr_{0.3}O_2$ materials were grown. For the Zr-doped films, Zr atoms are shown to occupy the lattice sites of Ce in the bulk structure of CeO_2(111). Also, oxygen storage characteristics of $Ce_{1-x}Zr_xO_2$ films will be discussed.