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X-ray photoelectron spectroscopy studies of $PrAlO_3$ crystals before and after thermal treatment

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Abstract

The as-grown $PrAlO_3$ single crystals grown by the Czochralski method are brown colored and after annealing in the reducing atmosphere (20%) H_2/N_2 they change the color to green. The X-ray photoelectron spectroscopy was used to study the chemical composition and electronic structure of $PrAlO_3$ single crystals before and after the thermal treatment. The core electron lines of praseodymium, aluminum and oxygen were measured and deconvoluted into the synthetic peaks to determine the chemical shifts. The mixed ionic and covalent character of bonds was found. The praseodymium valency may influence the coloration of the $PrAlO_3$ crystal. In the as-grown sample an additional Pr $3d_{3/2}$ peak at about 965 eV has higher intensity than that in the annealed one and is attributed to the presence of Pr^{4+} ions. The measurements showed the reduction of oxygen during thermal treatment and that interstitial oxygen was not removed in this process.