Growth, microstructure, and optical properties of high thermally stable wide-bandgap polycrystalline ferro-pseudobrookite FeTi2O5 sol-gel layers

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Wide band-gap and high thermal stability $FeTi_2O_5$ materials are promising for high temperature thermoelectric applications, green production of hydrogen by water splitting, fabrication of power electronics and optoelectronic devices.

High temperature stable wide-bandgap Fe-pseudobrookite, $FeTi_2O_5$, sol-gel coatings were grown on fused silica and (100)-Si substrates and characterised by thermal, morphological, microstructural, and optical analyses.[1] The experimental results show the formation of fractal-like patterns[2] where the $FeTi_2O_5$ layer covering the substrate have a compact structure, formed by close-packed crystallites (domain size ~16 nm) of pure, single phase orthorhombic $FeTi_2O_5$ which form at 560°C. Characterizations performed on annealed coatings (up to 950°C) show that the material remains in single $FeTi_2O_5$ phase up to a temperature of about 590°C. At higher temperatures, indeed, superficial Ti-O- dangling bonds begin to arrange themselves to form polycrystalline rutile-TiO_2 (crystalline domain size about 8 nm at 620°C), while the ferro-pseudobrookite phase remains unchanged. Moreover, as temperature increases above 750°C, the differences in the local chemical environments surrounding Ti and O atoms within the $FeTi_2O_5$ structure decrease, and the energy required to break the Ti-O-Ti molecular bonds increases. Optical spectroscopy measurements performed on coatings annealed at 560°C, yield an optical bandgap of about 2.25 eV, a refractive index of about 1.84 at 550 nm, and a UVC photoluminescence peak at about 5.6 eV; the latter feature disappears when the samples are annealed at 750°C, while the variation in the refractive index values and energy gap values is <5%.

***References**:*

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