PUBLICATION #1 :

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A new method for the determination of strain profiles in epitaxial thin films using X-ray diffraction

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Abstract

A new and versatile method is proposed for the determination of strain profiles in epitaxial thin films. It is based on the simulation of the X-ray diffraction (XRD) profiles using cubic B-spline functions to model the vertical lattice displacement profile. The lattice displacement profile, and consequently the strain profile, directly results from a least-square fit of the model to the experimental XRD profiles. No *a priori* assumption is made regarding the shape of the strain profile. Moreover, as spline functions are used, the recovered lattice displacement profile is smooth and exhibit a minimum curvature thus avoiding oscillating or saw-toothed unphysical solutions. The potential of this method is illustrated with (100) yttria stabilized zirconia epitaxial thin films deposited onto $(11\bar{2}0)$ sapphire substrates by sol-gel processing.

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Strain profiles in yttria stabilized zirconia epitaxial thin films determined by high-resolution x-ray diffraction

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Abstract

Epitaxial thin films of yttria stabilized zirconia (YSZ) have been grown onto $(11\bar{2}0)$ cut sapphire (Al_2O_3) substrates by sol-gel processing. The high crystallographic dissimilarity between YSZ and sapphire causes extremely high strains to build up at the interface. The microstructure of the samples has been investigated by high resolution X-ray diffraction using both a laboratory set-up and synchrotron radiation (ESRF, Grenoble). The strain profile across the film thickness has been recovered using a newly developed method that avoids assumptions regarding the shape of the strain profile.