Lab-based correlative X-ray imaging to study core formation and its impact on lattice uniformity in (Mg,Zr):$SrGa_{12}O_{19}$ single crystals

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We demonstrate the growth of large (Mg,Zr):$SrGa_{12}O_{19}$ (SGMZ) single crystals and use a combination of X-ray imaging techniques to analyze them structurally and chemically. Single crystal cylinders were obtained by top-seeded solution growth with optimized melt compositions. In the central parts of the grown crystals, we have observed stress-induced birefringence. As a possible explanation, we considered the formation of a small (0001) facet at the central part of the growth interface that should have a detectable impact on both the chemical composition and the crystal lattice. To test this assumption, we developed a quantitative rocking curve imaging technique (Fig. 1) with high sensitivity to study subtle variations of the microstructure.

This method enabled us to observe that the core region exhibits a reduced unit cell volume and is surrounded by a ring with increased lattice tilt and elastic strain. These effects were also analyzed using numerical simulations of the three-dimensional elastic stress and strain fields. Furthermore, variations of the cell volume in the outer parts of the crystal reveal a slight in-plane anisotropy of dopant incorporation following the hexagonal crystallographic symmetry. The relationship between unit cell dimensions and composition was verified by micro X-ray fluorescence mappings.

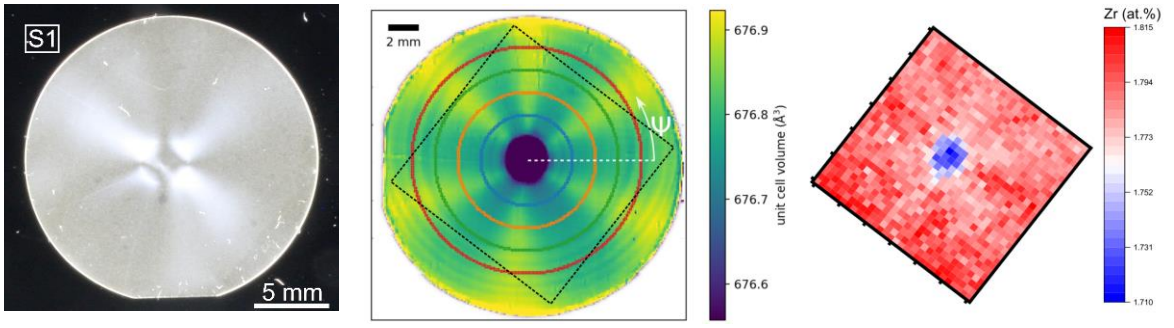

Fig 1: Determined maps of birefringence (left), unit cell volume (center) and Zr-fluorescence (right) of a 0001 cut SGMZ wafer.