XRD CHARACTERIZATION AND MODELLING OF EPITAXIAL PEROVSKITE $Pb(Zr_xTi_{1-x})O_3$ FILMS GROWN UNDER HYDROTHERMAL CONDITIONS

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Epitaxial PZT [$Pb(Zr_xTi_{1-x})O_3$] films ($x>0.5$) were synthesized on (100)-oriented $SrTiO_3$ substrates at temperatures from 150 to 300°C. The single-phase perovskite, continuous epitaxial layers were observed to be transparent under SEM, with the surface either atomically smooth or dominated by a screw dislocation-type or layered-growth morphology. Pole figures of the {013} planes showed excellent in-plane alignment on all films. Both symmetric and asymmetric reciprocal space maps of films 30-1100 nm thick showed overlapping broad (rocking curve FWHM ~ 0.5°) and narrow (rocking curve FWHM ~ 0.08°) peaks, which apparently represent at least two distinct layers of PZT of different crystal quality, thickness and structure. Changes in growth morphology, crystal quality, structure and lattice parameters were correlated with RBS data and XRD reciprocal space map measurements to generate a model for epitaxial perovskite film growth under equilibrium conditions.

XRD measurements were conducted using a Philips Analytical X'pert Materials Research Diffractometer System (Philips MRD) equipped with intermediate-resolution parabolic mirror optics collimating the incident and diffracted beams. This combination of optics produces a quasi-parallel and quasi-monochromatic X-ray beam with very high intensity and only a slight decrease in resolution from standard high-resolution optics. *Research supported by ONR, DARPA and the ONR AASERT Program.*