XRD, USAXS, SAXS and WAXS Investigations of ferroelectric PZN-4.5PT nanoparticles thin Films at APS synchrotron beamlines

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The $Pb(Zn_{1/3}Nb_{2/3})O3$-4.5$PbTiO_3$ (PZN-4.5PT) single crystals showed very large ferroelectric and piezoelectric properties compared to traditional ferroelectric ceramics ($BaTiO_3$ and PZT) used presently as active material in medical imaging, detection and sonars. However, despite these excellent properties, the greatest difficulty to use PZN-4.5PT single crystals on electronic devices is to achieve them in thin layers form because of their incongruent melting property. To overcome this difficulty, we deposit them as thin layers by dispersing their nanoparticles in a gel containing a matrix that can maintain at least their bulk properties. After this size reduction at nanoscale and the annealing process following the deposition, changes and structural transformations would occur. We fabricate with success thin films by dispersing these nanoparticles in a gel. The materials show some agglomeration at the surface of the silicon substrate films (from SEM images) and non-identified hexagonal microcrystals, which could be at the origin of their excellent properties.

In this paper we use the combined USAXS/SAXS/WAXS instrument at 9ID beamline at APSANL for in situ characterization of undoped and 1% Mn doped PZN-4.5PT inorganic perovskite nanoparticles thin films deposited on nanostructured silicon to understand the phases transitions and determine the observed hexagonal microcrystals structure. It revealed a hexagonal structure of the nanoparticles thin films, which could be explained by the new phase that can be assigned to the Pb3(PO4)2 based component. The peak at 31° indicates the presence of the rhombohedral phase perovskites assigned to the nanoparticles. XRD spectra, Raman and EDX mapping are compared to the USAXS, SAXS and WAXS results. WAXS characterization permitted to identify three phases transitions during thermal annealing confirming dielectric permittivity temperature phases transitions.

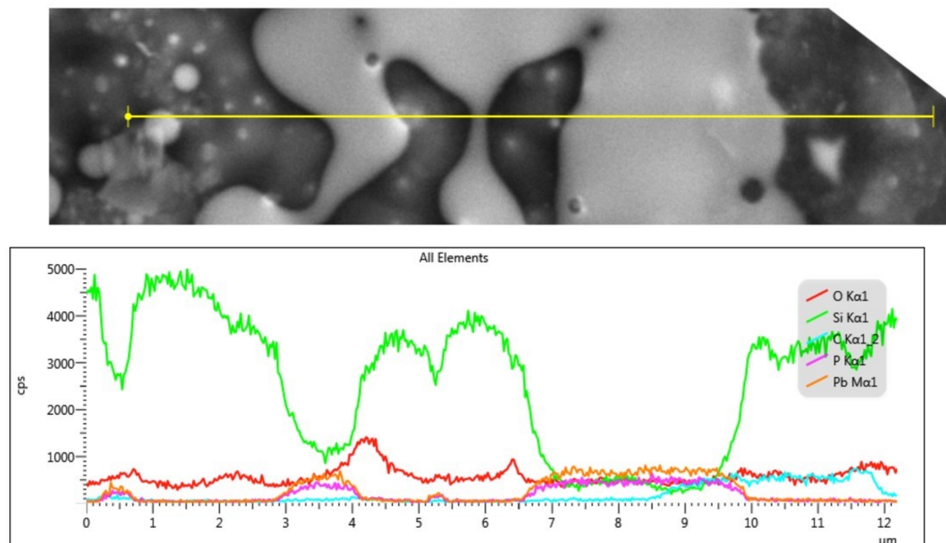

Figure 1: EDX mapping for PZN-4.5PT thin film on silicon substrate after annealing

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