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Structural Peculiarities of $0.67Pb(Mg_{1/3}Nb_{2/3})O_3–0.33PbTiO_3$ Thin Films Grown Directly on $SrTiO_3$ Substrates

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Abstract

Growth of $Pb(Mg_{1/3}Nb_{2/3})O_3–33PbTiO_3$ thin films by pulsed-laser deposition directly on non-conductive $SrTiO_3$ substrates for d_{33}-mode energy harvesters (EHs) was studied, as they offer a higher figure-of-merit than d_{31}-mode EHs. It was found that a high defect density, present in the film grown at 0.13 mbar, is manifested in the form of splitting of the (00*l*) peaks in X-ray diffraction, which was avoided by raising the process pressure to 0.27 mbar. Nevertheless, both films grow in a combined 2D and 3D manner, and form out-of-phase boundaries (OPBs) with a PbO rock-salt structure between the as-grown islands. It was found that the overall composition of the sample with optimized structural and functional properties was $Pb_{1.07}Mg_{0.19}Nb_{0.44}Ti_{0.32}O_3$, which is close to stoichiometric. The surplus of Pb is compensated by the formation of OPBs and Mg deficit maintains macroscopic electroneutrality. In-plane and out-of-plane relative permittivities of 1900 and 980, respectively, imply macroscopic out-of-plane polarization.

Keywords: pulsed-laser deposition, PMN-PT, crystal structure, piezoelectric thin films, Pb-loss compensation