Pyroelectric response of lead zirconate titanate thin films on silicon: Effect of thermal stresses

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J. Applied Physics, 114, Nov. 25, 2013

Abstract: Ferroelectric lead zirconate titanate [Pb(Zr x Ti1- x O)3, (PZT x:1-x)] has received considerable interest for applications related to uncooled infrared devices due to its large pyroelectric figures of merit near room temperature, and the fact that such devices are inherently ac coupled, allowing for simplified image post processing. For ferroelectric films made by industry-standard deposition techniques, stresses develop in the PZT layer upon cooling from the processing/growth temperature due to thermal mismatch between the film and the substrate. In this study, we use a non-linear thermodynamic model to investigate the pyroelectric properties of polycrystalline PZT thin films for five different compositions (PZT 40:60, PZT 30:70, PZT 20:80, PZT 10:90, PZT 0:100) on silicon as a function of processing temperature (25–800 °C). It is shown that the in-plane thermal stresses in PZT thin films alter the out-of-plane polarization and the ferroelectric phase transformation temperature, with profound effect on the pyroelectric properties. PZT 30:70 is found to have the largest pyroelectric coefficient (0.042 μC cm^{-2} $°C^{-1}$, comparable to bulk values) at a growth temperature of 550 °C; typical to what is currently used for many deposition processes. Our results indicate that it is possible to optimize the pyroelectric response of PZT thin films by adjusting the Ti composition and the processing temperature, thereby, enabling the tailoring of material properties for optimization relative to a specific deposition process.