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Compositional variation of thin PZT films near morphotropic phase boundary: experiment and simulation

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Extreme dielectric and electromechanical properties of PZT as well known can be observed in narrow band of solid solutions with a composition corresponding to the region of morphotropic phase boundary (MPB) (at x ≈ 0.46-0.48), that divides tetragonal and rhombohedral ferroelectric phases. In [1] it is assumed that such properties may be linked to the ferroelectric phase monoclinic modification existing in the region of MPB, which stability depends on element heterogeneity, microstructure and mechanical tensions. The search for compositions with most suitable electromechanical parameters involves accurate composition variation (Zr and Ti proportion) within the region of MPB. One of the ways to vary the multicomponent thin films composition is to control the technological parameters in the process of ion-plasma deposition and create directed flows of some components and diffusion flows of other components in target-substrate drift zone [2].

In this work, the study of coupling between variation of technological parameters of RF magnetron sputtering of ceramic PZT target (with elemental ratio Zr/Ti=54/46) and composition variation of deposited PZT thin layers was held. Two series of the samples were prepared. The first ones were formed under variation of the working gas pressure and the second ones - under variation of the distance between the target and the silicon substrate. To control thin-film compositions SEM EVO-40 (Carl Zeiss) equiped by energy-dispersive detector INCA was used. The films thickness was nearly 1 μm for the first series and nearly 0,5 μm for the second one. The experimental results on composition variation are presented in Figure 1a,b. The data of computer simulations of particles scattering in gas plazma have shown a good agreement with the experimental data.

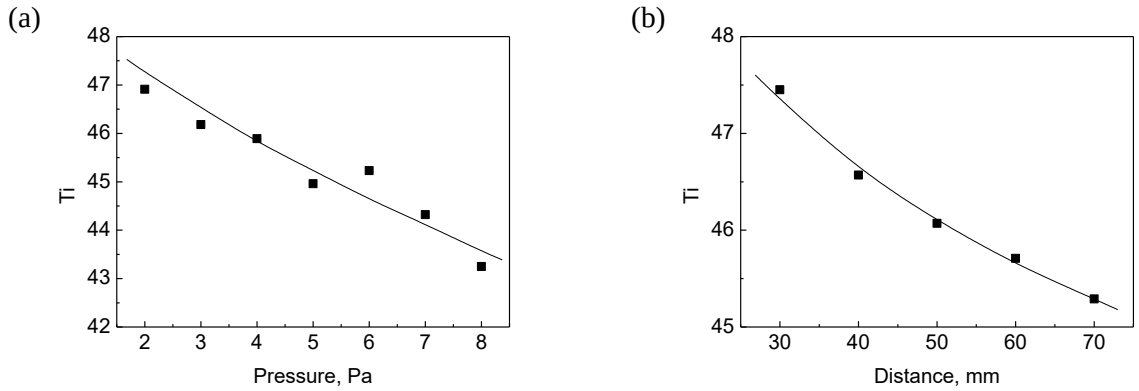

Figure 1. The change of thin PZT films composition versus the pressure of the working $Ar+O_2$ gas (a) and the distance between the target and the substrate (b).

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