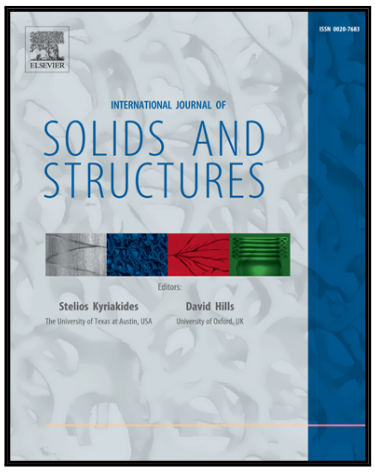

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PII: S0020-7683(18)30158-6
DOI: 10.1016/j.ijsolstr.2018.04.012
Reference: SAS 9967

To appear in: *International Journal of Solids and Structures*

Received date: 13 December 2017
Revised date: 27 March 2018
Accepted date: 11 April 2018

Please cite this article as: Qingnan Zhang , Xiaodong Xia , Jie Wang , Yu Su , Effects of epitaxial strain, film thickness and electric-field frequency on the ferroelectric behavior of $BaTiO_3$ nano films, *International Journal of Solids and Structures* (2018), doi: 10.1016/j.ijsolstr.2018.04.012

Effects of epitaxial strain, film thickness and electric-field frequency on the ferroelectric behavior of $BaTiO_3$ nano films

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Abstract

Ferroelectric nano films exhibit distinctive properties that are influenced by aspects such as the epitaxial strain, film thickness, and electric-field frequency. In this work, we studied the effects of the above factors on the ferroelectric behavior of $BaTiO_3$ nano films with a phase-field model based on the time-dependent Ginzburg-Landau kinetic equation. For the study of the epitaxial strain, we considered the cases with either compressive or tensile strain, ranging from -3.2 % to 1 %. Our results showed that the compressive epitaxial strain can generally enhance the remnant polarization and the coercive field, as opposed to the effect of the tensile one. As the film thickness reduces from 100 to 5 nm, the remnant polarization and the coercive field tend to increase, whereas the dielectric constant and the piezoelectric constant tend to decrease. We further investigated the effect of the high-strength electric-field frequency that varies from 0.1 to 100 kHz under two epitaxial-strain values, i.e., -0.1 % and -1.74 %, respectively. It was found that, at low frequencies, the coercive field increases sharply and the remnant polarization increases slightly with the rise of the applied frequency. Once the frequency gets higher than 20 kHz, the remnant polarization drastically reduces with the increasing frequency. In the meanwhile, the hysteresis loop exhibits an elliptic shape and the sharp tails of the butterfly loop are diminishing. We noticed that the frequency dependency is more sensitive to the epitaxial strain within the low-frequency range. Based on the obtained microstructural evolution process, we found that the 180° polarization reversal is more likely to occur under low-frequency field, while the polarization cannot be fully reversed in high-frequency hysteresis.

Keywords: Ferroelectric; nano film; phase field; epitaxial strain; size effect; frequency dependence

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