STRAIN ENGINEERING AND FERROELECTRIC BEHAVIOR OF $BaTiO_3$ THIN FILMS: A MOLECULAR DYNAMICS STUDY

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Low-dimensional perovskite-structured ferroelectrics display spontaneous polarization, piezoelectric and pyroelectric effects as well as large dielectric constants. They are candidates for numerous applications, such as ferroelectric memory (FeRAM), microsensors and micro- and nano-scale capacitors [1]. In these applications the properties of the devices are heavily dependent on the thickness of the ferroelectric layers, especially when approaching the scale of single atomic layers where the spontaneous polarization and hysteresis loop change considerably [2]. Barium titanate (BTO) is a model ferroelectric and researching it can provide insights into the mechanisms responsible for the thickness-dependance of ferroelectric properties [3].

This work is a continuation of the study [2], where vacuum-suspended BTO thin films were simulated using molecular dynamics package LAMMPS [4] and a core-shell model. The results showed that in thin films with thickness around 12 nm, in-plane polarized films exhibit a clear hysteresis loop, while out-of-plane polarized ones already exhibit other effects without a clear hysteresis loop.

The aim of this study is to expand of the previous results by including the effects of strain, which occurs in real devices, where ferroelectric layers are deposited on a substrate with a different lattice constant. One approach to simulating these effects is simulating a film, where the first few layers are fixed in place and the rest of the film relaxes on a ”stiff” base. This method shows, that the out-of-plane polarization of layers close to the base differs from the one for the suspended film and resembles it for layers further away. Other methods for simulating the substrate, such as applying additional external forces are also investigated.

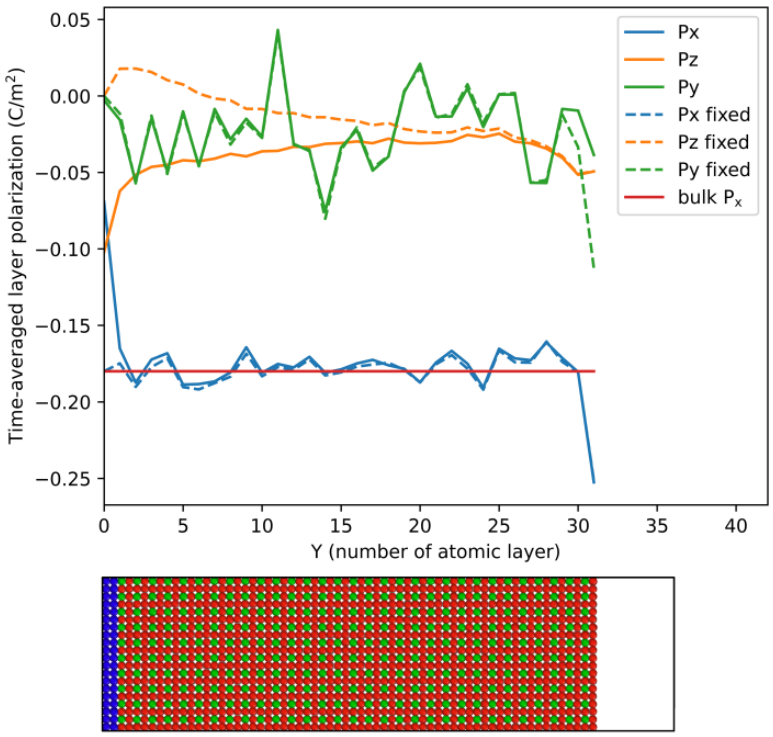

Fig. 1. The preliminary results of a polarization profile of a 12 nm film on a single fixed layer. z is the out-of-plane direction, the film is polarized in-plane. The structure below shows the fixed layers in blue, green represents barium, red oxygen and grey titanium.

[1] N. Setter, D. Damjanovic, L. Eng, et al.: Ferroelectric Thin Films: Review of Materials, Properties, and Applications, Journal of Applied Physics 100 (2006) 051606.
[2] A. K. Kushwaha, R. Khadka, P. Keblinski, Surface-Induced effects in ferroelectric BaTiO3 thin films, Surfaces and Interfaces 56 (2025) 2468-0230
[3] R. Khadka, P. Keblinski: Molecular dynamics study of domain switching dynamics in KNbO3 and BaTiO3. Journal of Materials Science 57 (2022) 12929–12946
[4] Aidan P. Thompson et al. LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales, Computer Physics Communications 271 (2022) 0010-4655