Non-linear switching kinetics of ferroelectric mono-domain single crystals

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ABSTRACT

Understanding the electric polarization switching kinetics in ferroelectric materials is critical to many applications such as fast high-density non-volatile random access memory devices [1]. Experimental studies of the domain switching process in bulk and thin film ferroelectrics under an external electric loading have explained the switching kinetics using the Kolmogorov-Avrami-Ishibashi (KAI) model. The KAI model is based on the classical approach of nucleation and subsequent growth of reversed domains [2]. It describes the time-dependent normalized change in polarization as a Lorentzian function [3].

We perform molecular dynamics simulations to investigate the electric polarization switching kinetics of mono-domain ferroelectric $BaTiO_3$ single crystals under external electric loading at room temperature using the core-shell model. In the core-shell model every ion is represented in terms of a charged core and a charged electron shell which introduces electronic polarizability in the ions. We study the polarization switching process with atomistic detail and discuss the applicability of KAI model in explaining the non-linear polarization switching kinetics of mono-domain ferroelectric perfect single crystals.

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