Interplay of domain structure, phase transitions and functional responses in ferroelectric $BaTiO_3$

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Domain walls and phase boundaries are fundamental ingredients of ferroelectrics and govern their functional properties important for applications ranging from frequency conversion, energy harvesting, electrocaloric cooling and piezoelectric actuation to data storage. Although both interfaces have been studied for decades, often only a phenomenological macroscopic understanding has been established and recent studies reveal unexpected microscopic properties [1].
In this talk I will discuss how domain walls in the tetragonal and orthorhombic phases of $BaTiO_3$ may improve the functional properties in films with strain gradients [2] and reduce thermal hysteresis of phase transitions [3]. Furthermore, I will discuss our recent findings on the field-coupling of 180° domain walls [4]. All results have been obtained by ab-initio based molecular dynamics simulations [2].

Literature

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