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Analytical Description of Size Effects, Strains and Ferro-ionic Coupling in Si-Compatible Nanosized Ferroelectrics

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The analytical methods based on the Landau-Ginzburg-Devonshire (LGD) approach and variational principle allow the analytical description of size effects, strain and ferro-ionic coupling in low-dimensional ferroelectric materials, such as thin films and small nanoparticles. The validity of LGD approach is corroborated by experimental evidence of the size- and strain-induced transitions as well as the related phenomena in the low-dimensional ferroelectric materials. For the correct description of these effects in ferroelectric thin films and small nanoparticles the LGD approach should be combined with the classical electrostatics and elasticity theory, and variational principle. It is important to determine how the LGD expansion coefficients depend on various factors, such as temperature, size, elastic stresses and/or strains, and ionic-electronic charge density and distribution. For classical ferroelectric films with a pronounced temperature-dependent and strain-dependent soft mode, the first expansion coefficients have a linear dependence on the temperature and elastic strain.
The significant attention is devoted to the comparison with experimental results and finite element modelling, as well as on the theoretical predictions of the size-, strain- and ionic- control of polar and dielectric properties of nanosized ferroelectric materials.
As the first example, we consider ultra-thin layers and nanoflakes of van der Waals ferrielectric CuInP2S6 covered by an ionic surface charge and reveal the appearance of polar states with relatively high polarization and stored free charge, which can mimic "mid-gap" states related with a surface field-induced transfer of Cu and/or In ions in the van der Waals gap [1]. The changes of the ionic screening degree and mismatch strains can induce the transitions between paraelectric phase, antiferroelectric, ferrielectric, and ferroelectric-like states in CuInP2S6 nanoflakes. Due to the emergence of manyfold-degenerated metastable states of spontaneous polarization the ultra-thin layers of CuInP2S6 reveal features of the controllable negative capacitance effect [2], which make them attractive for advanced electronic devices, such as nano-capacitors and gate oxide nanomaterials with reduced heat dissipation.
As the second example, we use the LGD model to quantify the strain-charge-polarization coupling in nanosized HfxZr1-xO2. A key factor ruling the observed polar properties of nanosized HfxZr1-xO2 is the presence of the polar orthorhombic phase. This phase is metastabile compared to the bulk monoclinic phase, leading to problems with the ferroelectric phase stability in nanoscale. The electrophysical properties of the HfxZr1-xO2 thin films and nanoparticles are very sensitive to the elastic strain induced by the substrate, annealing conditions, deposition method, film thickness, content x and dopants. Depending on the interplay of these factors, the nanosized HfxZr1-xO2 exhibits dielectric, ferroelectric, or antiferroelectric behavior.
The used model [3] incorporates parametrized Landau expansion coefficients for the polar and antipolar orderings. Obtained results agrees with the recent existing experimental data for HfxZr1-xO2-y thin films and oxygen-deficient HfO2-y nanoparticles [4], namely the X-ray diffraction confirmed the formation of a ferroelectric orthorhombic phase in the HfO2-y nanoparticles under special favorable annealing conditions.
The analytical LGD approach correctly predicts the phase diagrams, ground and metastable states, alongside the domain structure morphology, associated polar and structural properties of HfxZr1-xO2-y thin films and nanoparticles with different shapes and sizes. The successful application of the analytical LGD approach can be useful for the prediction of the silicon-compatible ferroelectric nanomaterials based on HfxZr1-xO2-y.
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