Topology of the ferroelectric polarization at the $BaTiO_3$(001) surface from ab initio calculations and electron microscopy-spectroscopy

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The polarization discontinuity at a ferroelectric surface induces fixed charge which can destabilize the ferroelectric state. Domain ordering naturally screens the depolarizing field and maintains the ferroelectric stability. At the surface of ferroelectric oxide, domain patterns combine with atomic rearrangement to minimize the total free energy of the system. As a result, the combination of domain ordering and atomic reconstruction and relaxation is expected to give rise to specific surface ferroelectric topologies.

In this thesis, first principles calculations using density functional theory have been performed to explore the role and interactions of surface termination, strain, thickness, oxygen vacancies and domain width on the ferroelectric topology of ultrathin $BaTiO_3$(001) films. The theoretical results are compared with low energy electron and photoelectron emission microscopy studies of $BaTiO_3$(001) single crystal surfaces. The specific role of the surface chemistry and structure appears key in determining the ferroelectric topology.