

Effect of dislocation walls on the polarization switching of a ferroelectric single crystal

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Phase field simulations were conducted to study the influence of dislocation walls on the domain configuration and hence the polarization switching behavior of a ferroelectric single crystal. The simulation results show that when Dislocation Line Density (DLD) is high, unusual 90° domain walls exhibit along the dislocation walls and the conventional twin domain structure without dislocations changes to a mixed 90° and 180° domain structure. The polarization switching behavior depends highly on the DLD. This study indicating that introducing an appropriate dislocation density at high temperature improves the ferroelectric properties. The phase field simulations also put insights into the mechanism of polarization switching.

Key Words: *Phase field simulation, Ferroelectrics, Dislocation wall, Temporal evolution*