## Influence of coherent twin grain boundary on domain configuration in PZT

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Defects are important for the studying of ferroelectric materials, since they can induce local electric and elastic field. These pinning sites for domain wall migration will further cause the nonlinearity response under electric field. [1] Before diving into the research of switching behavior, it is meaningful to learn what domain pattern is most stable at the presence of a grain boundary, and why such type of configuration is more favorable. Some recent experiment results show domain characterization in vicinity of the grain boundary with great quality. [2] In this work, the simplest type of grain boundary, the coherent twin boundary, was introduced and studied using the time dependent Landau-Ginzburg phase field model. The composition we simulated is Pb(Zr0.2Ti0.8)O3, which has a tetragonal low temperature ferroelectric phase. Three different domain configurations were examined as it is shown in figure 1, exploring the effect of low and high angle, as well as the effect of aligned and unaligned domains. Result shows that the stress state at the grain boundary plays a vital role in stabilizing certain type of bordering domains. For example, due to the asymmetric geometry between partial head to head and partial tail to tail domains at the grain boundary, the previous one is more favored than the latter one.



Figure 1 Three initial domain configurations.

## References

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