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Molecular dynamics study of ferroelectric 90 degree domain walls in lead titanate[1] TINGTING QI, JACOB COLBERT, I-WEI CHEN, ANDREW RAPPE, THE MAKINENI THEORETICAL LABORATORIES, DEPARTMENT OF CHEMISTRY, UNIVERISTY OF PENNSYLVANIA COLLABORATION, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, UNIVERSITY OF PENNSYLVANIA COLLABORATION — Molecular dynamics (MD) simulations were carried out to study the 90° domain wall dynamics of $PbTiO_3$ under mechanical strain. By using a well-parameterized interatomic potential, the rate of formation of new 90° domains at different temperatures and strain states were extracted. Due to faster stress relaxation, the nucleation rate is slower and the critical nucleus larger at higher temperature. Furthermore, alternative stress relief mechanisms are studied. The critical nucleation size is found to be small. A simple mathematical model describing the relationship between rate and strain is formulated.

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