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Interplay of the strain and microstructure in ferroelectric epitaxial CaTiO3 Films[1] QIAN HE, QIAO LIANG, MICHAEL BIEGALSKI, ALBINA BORISEVICH, Oak Ridge National Laboratory — CaTiO3 (CTO) was predicted to become ferroelectric under lattice strain. However, other factors such as oxygen octahedral tilts or microstructural details can play a role. In this work, two 20 nm CTO films were grown on LSAT and NGO by PLD. They both show ferroelectricity, with Tc near 140 K on LSAT and near 70 K on NGO, and the remnant polarization at 10K of 5 and 2 μC/cm, respectively. This is surprising given that the strain of CTO on both substrates is similar. AC-STEM shows two major differences in microstructure between two CTO films: Firstly, the first few nm of CTO on NGO show perfect epitaxial growth, and after that grains start to develop, but the c-axis of CTO remains aligned with the c-axis of NGO, suggesting the presence of 180° grain boundaries only. However for CTO/LSAT, grains begin to develop at the interface and their c-axes have two possible orientations, resulting in both 180° and 90° grain boundaries. These grain boundaries are either dislocations or ferroelastic twins. Secondly, the octahedral tilt behavior at the film/substrate interface is different: CTO/LSAT has a 5-6 unit cell transition region from the untilted LSAT to the tilted CTO, which is not the case in CTO/NGO. The connection between the microstructure, substrate strain and connections to the ferroelectric properties will be discussed in detail.

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