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Structure of $SrTiO_3$ films on Si C. STEPHEN HELLBERG, Naval Research Lab, KRISTOPHER ANDERSEN, High Performance Technologies, Inc., HAO LI, Shenzhen New Degree Technology Co., PHILIP RYAN, Argonne National Laboratory, JOSEPH WOICIK, National Institute of Standards and Technology — The epitaxial deposition of oxides on silicon opens the possibility of incorporating their diverse properties into silicon-device technology. Deposition of $SrTiO_3$ on silicon was first reported over a decade ago, but growing the coherent, lattice-matched films that are critical for many applications has been difficult for thicknesses beyond 5 unit cells. Using a combination of density functional calculations and x-ray diffraction measurements, we determine the atomic structure of coherent $SrTiO_3$ films on silicon, finding that the Sr concentration at the interface varies with the film thickness. The structures with the lowest computed energies best match the x-ray diffraction. During growth, Sr diffuses from the interface to the surface of the film; the increasing difficulty of Sr diffusion with film thickness may cause the disorder seen in thicker films. The identification of this unique thickness-dependent interfacial structure opens the possibility of modifying the interface to improve the thickness and quality of metal oxide films on silicon.

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