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Formation of Alkaline Earth Template Layers for Oxide Epitaxy on Semiconductors: Surface Alloying and Self-Organization BORIS LUKANOV, KEVIN GARRITY, JAMES REINER, FRED WALKER, SOHRAB ISMAIL-BEIGI, ERIC ALTMAN, Yale University — The finding that Sr and Ba titanates can be grown epitaxially on Si and Ge (100) surfaces without oxidizing the semiconductor and with atomically abrupt interfaces, has spurred research into exploiting these materials for high-k gate dielectrics and for integrating new functionality into traditional semiconductor devices. To date, all successful oxide eptiaxy on Si and Ge (100) surfaces has required the initial formation of a sub-monolayer of an alkaline earth metal. To understand how this layer promotes oxide epitaxy, we have been using scanning tunneling microscopy complemented by electron diffraction and density functional theory to characterize the formation of the template layer on the atomic scale. The results reveal a complex series of phase transitions as Sr is deposited onto Ge(100). Interestingly, each phase transition is accompanied by drastic changes in the surface morphology that can only be explained by formation of an alloy surface. Through comparison of atomic-resolution STM images with DFT predictions, structural models of two of the surface alloy phases have been deduced. Incorporation of the larger alkaline earth atoms into the surface creates strain that is ultimately relieved by the formation of remarkably well-ordered arrays of stripes and trenches. The alloy formation leads to double-height steps on the surface, resulting in unidirectional trenches and nanowires extending for thousands of Angstroms.

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