

Phase Diagram of Sr on Si (100): a first-principles study

K. F. Garrity, J. W. Reiner, F. J. Walker, C. H. Ahn, and S. Ismail-Beigi

*Departments of Physics and Applied Physics, Yale University
New Haven, Connecticut, USA*

As transistors continue to get smaller and faster, all of their components must scale down accordingly. In particular, current technology requires a dielectric layer which is only a few angstroms thick. Due to quantum mechanical leakage currents at these dimensions, new materials with higher dielectric constants and good interfaces with silicon are required in order to continue this scaling process. More generally, the epitaxial integration of complex oxides with semiconductors would allow new devices which take advantage of the wide range of oxide properties, including ferroelectric, ferromagnetic, piezoelectric, and multiferroic behavior.

To date, the only known method to grow complex oxides on silicon epitaxially has required 1/2 ML of Sr to be deposited as a first step. As the Sr is deposited under normal experimental conditions, transitions from a 2x1 silicon reconstruction to a 2x3 and then to a 1x2 phase are observed. These transitions were thought to be required to achieve good epitaxy, but their origin and significance has not been understood.

Using first-principles density functional theory calculations, we examine the growth of sub-monolayer coverages of Sr on Si (100) and explain the unusual phase diagram observed experimentally. In particular, we look at a novel class of 1/6 ML structures which require the replacement of 2/3 of the surface silicon dimers. These new structures explain both the reconstructions seen at 1/6 ML as well as the rotation of the surface silicon dimers which is observed during high-temperature Sr deposition. We also predict the successful growth of oxides under low-temperature conditions with the same interface structure as in the high-temperature case, but rotated 90 degrees.

In order to understand the 1/6 ML structures better, we employ maximally-localized Wannier functions to examine their unusual bonding.