

Reconstructions and nanostructures on strontium titanate surfaces: scanning tunnelling microscopy and ab-initio modelling.

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SrTiO₃ is traditionally used in thin film form to exploit its high dielectric constant. More recently it has found application as an alternative gate dielectric material to replace SiO₂ and also as a buffer material for the epitaxial growth of GaAs on Si. We have used scanning tunnelling microscopy (STM) to elucidate the nature of the SrTiO₃ (001) and (111) surfaces as well as observing the spontaneous growth of surface nanostructures. We believe the nanostructures to be due to local phase separation caused by non-stoichiometry in the surface region.

As a result of STM and other techniques a number of atomic structure models have been proposed for the reconstructions on SrTiO₃ (001). By running ab-initio calculations for a variety of (1x1) and (2x1) structures we are able to show which structures are stable under which conditions. The ab-initio modelling is also used to show the surface density of states which in turn feeds back into STM image interpretation.

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