Structural relaxation at interfaces of transition metal oxides

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In complex heterostructures of transition metal oxides, interface phenomena can lead to novel electronic states not observed in the bulk constituents. For several types of oxide heterostructures, we have studied interface discontinuities due to the lattice mismatch with the substrate and the effects of interface polarity. We have found that structural discontinuities induce a new type of a mixed electronic-lattice reconstruction near the interface which include: (1) the modification of lattice constants and local static atomic displacements in the interfacial region, and (2) a reconstruction of the state of the electron subsystem. One of the example of the considered reconstructions is the metal-insulator transition in the heterostructure of $LaAlO_3$ film and $SrTiO_3$ observed upon the increase of the film thickness. Another mixed process known as orbital reconstruction is related to a change in orbital occupations of the transition metals near the interface which can be activated by structural relaxation. A comparison of the results obtained for oxide interfaces with the experimental studies by scanning tunneling spectroscopy shows a key role of the local Coulomb repulsion in the interfacial electronic properties. As a result, the electronic system at the interface of the oxide heterostructure is not a two-dimensional electron gas (2DEG), but can be described as a two-dimensional electron liquid (2DEL), a new interfacial state recently revealed at titanate-lanthanate interfaces. Interfaces in oxides therefore broaden the spectrum of available two dimensional electron systems from the 2DEGs of conventional semiconductors to also include two-dimensional systems with strong electronic correlations.