Chapter 11
Application to prototypical metal-oxide clean surfaces: the complex TiO_2 (110) surface reconstruction

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Metal-oxide surfaces are structurally complex systems due to a variety of stoichiometries. Furthermore, different structures can exist for one particular chemical composition and presence of defects. Also, oxide surface depends sensitively on preparation conditions with limited possibility of annealing and purification afterward, making it difficult to arrive at the thermodynamical optimum. Therefore, compared to metals or semiconductors, where high structural quality of the surfaces can be achieved, oxide surfaces are not that well defined in terms of stoichiometry and imperfections. This suggests that the standard surface structure simulation approaches, based on periodically repeated supercell, might not provide the correct total energy minimum. As a consequence, simulated surface atomic geometry might not accurately describe the experimental surface structure of the oxides. Therefore, we will only briefly refer to a few theoretical or review papers on the oxide surfaces without presenting atomic structure model and structural tables.

Titanium dioxide TiO_2 is a very important oxide material with its surfaces being intensively investigated. However, the theoretical and experimental results for a variety of structures do not generally agree well. The reason is that often, the surface contains a mixture of different structures and stoichiometries, and they always have a lot of defects (see, e.g., [94Hen, 96Fre, 03Die, 10Die]). For the relaxed geometries, we can refer to TiO_2(110) surface [03Die] (Table 3 on p. 72) or detailed comparison of STM and ab initio simulation [07Par] (Tables 1 and 2). Other examples can be technologically important ZnO surfaces, which have been also studied recently [08Du, 13Pal]. Both TiO_2 and ZnO surfaces contain a lot of defects, such as islands and pits of various sizes that can be understood from the formation energies' point of view. In view of the above complexity when interpreting experimental results on surfaces of oxides, we do not go in further details of the simulated surface atomic structures.

Symbols and abbreviations

Short form	Full form
STM	scanning tunneling microscopy

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