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Oxygen-Induced Faceting of Ir(210) TIMO JACOB, PAYAM KAGHAZCHI, MATTHIAS SCHEFFLER, Fritz-Haber Institute, Faradayweg 4-6, D-14195 Berlin, Germany — Although rough clean metal surfaces usually have higher surface free energies than their closed-packed analogs, adsorbates are able to modify this behavior and cause changes in surface morphology through reconstructions or facet formations. Using different surface sensitive techniques (e. g. STM or LEED) Madey *et al.* [1] found that Ir(210) shows interesting surface faceting at high oxygen coverages ($\theta > 0.5$ ML). The facets were identified as three-sided nanoscale pyramids with two (311) and one (110) planes. In order to understand this effect we used density functional theory in combination with the *ab initio* atomistic thermodynamics and studied the influence of an oxygen atmosphere on the structure of Ir(210). Assuming an oxygen partial pressure of 1 atm, it turned out that below $T < 1000$ K the oxygen-covered facets are thermodynamically more stable than non-faceted O/Ir(210). Further heating reverts the substrate structure to planar O/Ir(210). While most nanoscale pyramids consist of smooth and unreconstructed planes, some (110) facets show a complex reconstructed superstructure. Thus, present studies aim on the stability and an atomistic understanding of those structures.

[1] I. Ermanoski *et al.*, *Surf. Sci.* **549**, 1 (2004).

Timo Jacob
Fritz-Haber Institute, Faradayweg 4-6, D-14195 Berlin, Germany

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