Surface oxides on $Pt_3Sn(111)$

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Platinum-tin alloys are employed as components of efficient electrocatalysts for e.g. alcohol oxidation [1] as well as active catalysts for preferential CO oxidation in hydrogen [2], and as such are useful materials for application in fuel cells, among other technologies. The formation of oxides—especially of tin—during reaction conditions is believed to significantly affect the catalytic properties of this material, in certain conditions leading to dramatic increases in activity [3].

The aim of the current project is to elucidate the nature of the oxides formed at Pt-Sn alloy surfaces and their structure at the atomic scale, and to link this to the materials' catalytic properties. As a first step in this direction, we have studied the initial oxidation of a $Pt_3Sn(111)$ single crystal surface under UHV conditions using scanning tunnelling microscopy (STM), surface X-ray diffraction (SXRD) and density functional theory (DFT) calculations. The oxidation process is found to involve extraction of Sn from the surface layer and assembly of 2D surface oxides with different morphologies depending on the oxidation temperature (see Fig. 1). We present here the detailed characterization of these phases by STM as well as the results of recent SXRD measurements and DFT calculations performed with the goal of elucidating the atomic structure of the well-ordered (4x4) phase. The results are discussed in relation to previous experiments on this surface [4] and to the surface structures of bulk tin oxides, such as the recently-solved $SnO_2(110)$-(4x1) phase [5].

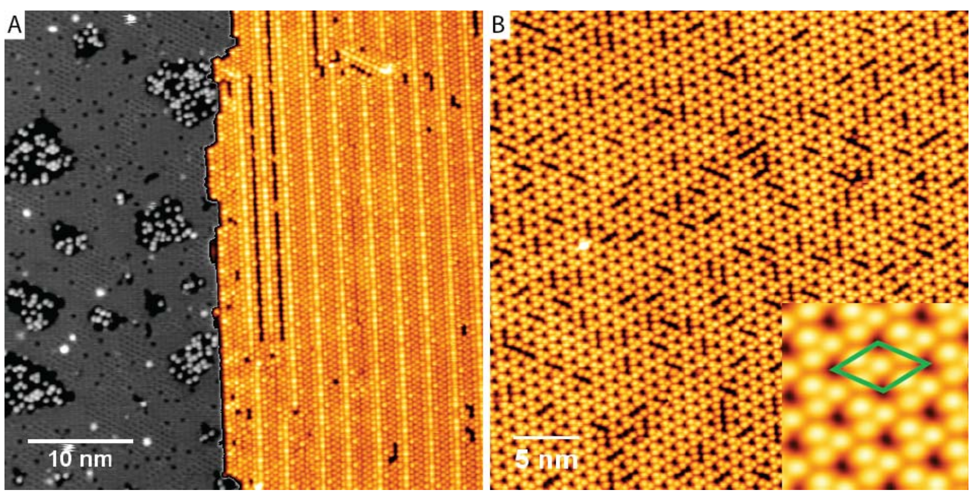

Figure 1. STM images of different surface oxide phases formed at the surface of $Pt_3Sn(111)$. A) Surface immediately following oxidation between 400 and 500˚C. Removal of Sn results in formation of distinct pits in the metal surface, seen at left, with the 2D surface oxide growing at right, in the form of a partially-ordered 'striped' phase. B) Post-annealing or oxidation at higher temperatures leads to formation of a well-ordered "(4x4)" phase. Inset: detail of the structure obtained by Fourier averaging.

References:
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