Reaction driven ordering of the surface of an alloy PtRh model catalyst

Helen Edström[a], Uta Hejral[a], Stefano Albertin[a], Kim von Allmen[a], Benjamin Hagman[a], Edvin Lundgren[a], Andreas Schaefer[b], Andreas Stierle[c], Vedran Vonk[c], Christoph Seitz[c], Simon Geile[c], Ulrich Lienert[c], Timo Müller[c], Zoltán Hegedűs[c], Sven Gutschmidt[c], and Johan Gustafson[a]

[a]Synchrotron Radiation Research, Lund University, Box 118, SE-221 00 Lund, Sweden, [b]Department of Chemistry and Chemical Engineering, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden, [c]Deutsches Elektronen-Synchrotron (DESY), D-226 03 Hamburg, Germany

helen.edstrom@sljus.lu.se

Since exhaust from automotive engines contains a number of toxic pollutants, a catalyst is needed to transform them into less harmful substances. Such a catalyst often consists of Pt and Rh, and combining them in a bimetallic alloy could be advantageous. In a PtRh alloy, there is a synergy between the two metals when it comes to CO oxidation: Pt is more active under strongly oxidizing conditions, while Rh is more active under reducing conditions [1]. Though this alloy system is extensively studied, it is not completely understood. To better understand what happens on the surface of the PtRh alloy during catalytic reactions, we performed CO oxidation on a $Pt_{25}Rh_{75}$(100) single crystal under varying reaction conditions, while studying it with high-energy surface X-ray diffraction (HESXRD).

We observed three different surface structures. Two of them were expected: a p(3×1) reconstruction with chemisorbed O under mildly oxidizing conditions and a c(8×2) surface oxide under strongly oxidizing conditions [2]. Under reducing conditions and elevated temperature, we further found a c(2×2) surface structure, which remained even when returning to strongly oxidizing conditions. Figure 1a shows the HESXRD intensity as a projection in the h-k plane, where the rods seen at (h, k) = (0.5, 0.5) and (0.5, 1.5) reveal the c(2×2) superstructure. CO has been found to adsorb in atop sites in a c(2×2) structure on both Pt(100) [3] and Rh(100) [4], and thus we would expect CO to adsorb on PtRh(100) in the same way. However, our analysis indicates that the c(2×2) structure originates not only from the adsorbed CO. Figure 1b shows how the structure factor varies along the superstructure rods. The first peak appears at $q_\perp$ = 1 Å^{-1}, corresponding to a maximum out-of-plane distance of atoms contributing to the c(2×2) structure of 6 Å. This would approximately correspond to the distance between the O atom of the adsorbed CO and the third metal layer, as illustrated in Figure 1c.

In this contribution we will discuss the current status of the analysis and the concequences of the results.

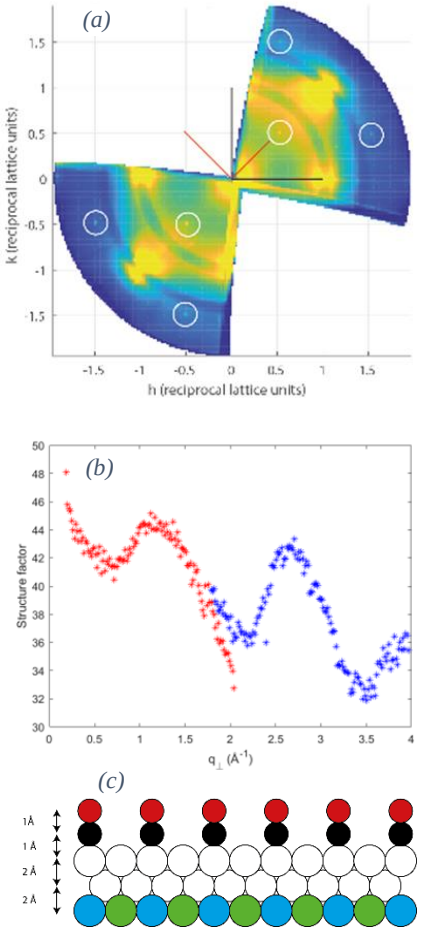

Figure 1. (a) The HESXRD intensity shown as a projection in the h-k plane. The white rings indicate the c(2×2) rods. (b) The structure factor as a function of q value for the c(2×2) rods. (c) Sideview of the first three metal layers and the adsorbed CO molecules.

References

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