International Workshop on Nanostructured Materials, NANOMAT 2006, Antalya, Turkey, 21.-23. June 2006
Invited talk

Surface science meets catalysis research: epitaxial iron oxide films for in-situ model catalysis

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Abstract

I will review a fairly successful attempt to bridge the gaps between surface science studies and real catalysis for the case of ethylbenzene (EB) dehydrogenation to styrene (St) over unpromoted and K-promoted iron oxide catalysts. Epitaxial films of Fe_3O_4(111), α-Fe_2O_3(0001), $K_xFe_{22}O_{34}$ and $KFeO_2$ were prepared and characterized using surface science methods. Their catalytic behavior was studied after vacuum-transfer in a micro flow reactor, followed by post-reaction surface analysis. The results are : (i) Defects are necessary for the dehydrogenation step; (ii) most active is Fe^{3+} in Fe_2O_3 or KFe_xO_y; (iii) unpromoted catalysts deactivate by reduction to Fe_3O_4 and by coking; (iv) both can be prevented by some oxygen in the feed; (v) K is catalytically inactive but suppresses reduction and catalyses carbon removal; (vi) $K_2Fe_{22}O_{34}$ and $KFeO_2$ are K-reservoir phases; (vii) "steaming" (reaction in steam without EB) exhausts the K-reservoir phases; (viii) coke has non-zero catalytic activity and contributes to conversion in real catalysis. In cooperation with the ICVT in Stuttgart, microkinetic modelling was performed aiming at a prediction of the behaviour of technical catalysts. Using physically meaningful parameters, mostly determined in surface science experiments, an excellent fit was achieved which could even be extented to porous samples.