GdCh-Jahrestagung 2003
6.-11.10.03
München / Deutschland

Structural and Catalytic Investigation of Binary Palladium-Gallium Alloys

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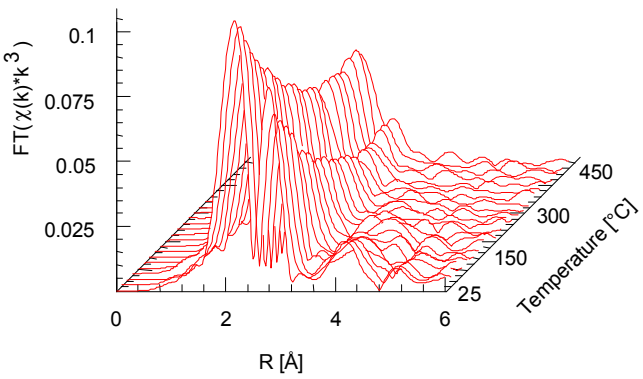
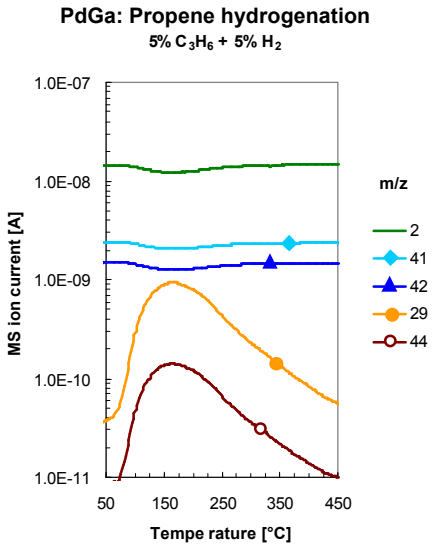
Palladium is well-known as an important catalyst for hydrogenation and for combustion reactions[1]. Typical Pd-catalysts are supported on metal oxides and shows high activity but only limited selectivity. The limited selectivity of Pd catalysts is due to neighbouring active sites on the catalyst metal surface[2]. From this it follows that active site isolation may increase selectivity.
The binary alloys PdGa and Pd_3Ga_7 are stoichiometric compounds with ordered structures. These materials are particularly interesting as possible catalysts due to isolation of the Pd atoms in the structure. In both structures the Pd atoms are surrounded by a closed coordination sphere of Ga atoms (i.e. coordination number of 7 in PdGa and 8 in Pd_3Ga_7). Conversely a supported Pd catalyst presents an ensemble of neighbouring Pd atoms to the reactants. This significant difference in structures between Pd metal and the alloys may provide a unique selectivity.
We investigated the thermal stability of these alloys in the presence of various atmospheres with *in situ* XAS on both the Pd and the Ga K-edge and also with complementary methods *in situ* XRD and thermal analysis. We determined the bulk behaviour of the alloys in helium, hydrogen and oxygen from temperatures from 293 to 593 K.
First catalytic studies show activity for propene hydrogenation and partial oxidation to acrolein as well as high selectivity for acetylene hydrogenation to ethylene.





The radial distribution function of PdGa in propene and hydrogen (left) and the corresponding MS diagramm with the masses 41+42 for propene and 29+44 for propane (right).

Literature:
[1]G. Ertl, H. Knoezinger, J. Weitkamp: Handbook of heterogeneous catalysis, VCH, 1997
[2]A.J. Den Hartog, M. Deng, F. Jongerius, V. Ponec, J. Mol Catal. 60 (1990) 99