

PROJECT FACTS

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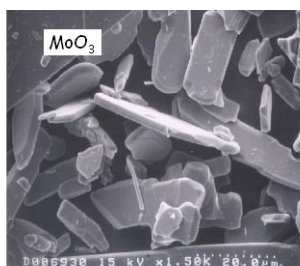
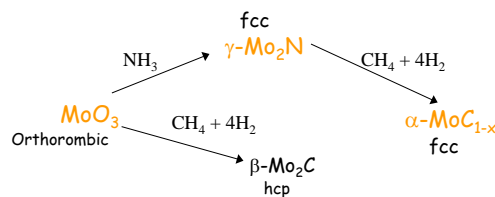
CLEAN FUELS & CHEMICALS

Transition Metal Carbides in Fischer-Tropsch Synthesis

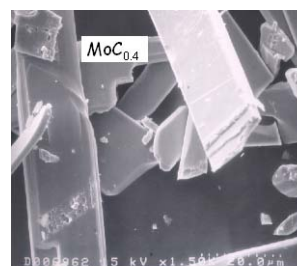
Iron is one of the most widely used catalysts for the Fischer-Tropsch synthesis and it is commonly accepted that one of its many carbide forms is the catalytically active component. The iron carbides are produced *in situ* by pretreatment of iron oxide precursors using the synthesis gas itself. Other transition metal carbides, such as those of molybdenum and tungsten, have demonstrated significant catalytic activity in chemical reactions normally catalyzed by noble metals. In particular, molybdenum carbides (either hexagonal or cubic, both of which have the empirical formula Mo_2C) compare very favorably with Ru catalysts for hydrogenation or hydrogenolysis reactions. The reason for the enhanced activity when compared with the parent metal can be explained in electronic terms. Le Sabatier in his oft-quoted Principle stated that "A most important property of an excellent catalyst is its ability to bind many organic and inorganic molecules strongly enough but not too strongly". The insertion of carbon into the Mo lattice causes it to expand with a subsequent contraction of the d-band. Thus, even with fewer electrons, the band is filled to a greater extent and the density of states at the Fermi level will be equivalent to that of the Group VIII noble metals, and high metal catalytic activity correlates with a high density of states at the Fermi level.

The group of M. Boudart developed a temperature programmed reaction for Mo_2C synthesis which led to high specific surface area bulk carbides, thus increasing the interest in these species as catalysts. The process involves heating the parent MoO_3 slowly in a controlled manner according to the scheme outlined below. The final product depends on the conditions employed. Surface areas of 50 to 100 m^2/g for the hcp carbide and up to 200 m^2/g for the fcc nitride and carbide have been obtained. The process by which the oxide is converted to the fcc carbide is a topotactic one whereby the morphology of the parent compound is retained in the final product as can be seen in the SEM images below.

Because of the comparable catalytic activity of these compounds to Ru (another well known FTS catalyst), we are currently testing them for FTS activity in the Continuously Stirred Tank Reactors here in the CAFR



SEM image showing platelet morphology of parent molybdenum oxide



SEM image showing platelet morphology of product molybdenum carbide