Preparation of single crystalline iron carbide model catalysts for syngas conversion via the Fischer-Tropsch synthesis.

García R. Daniel[1], Weststrate. C.J.[2]

[1]*DIFFER, De Zaale 20, Eindhoven, NL*
[2]*Syngaschem BV, De Zaale 20, Eindhoven, NL*
d.garciarodriguez@differ.nl

Fischer-Tropsch synthesis (FTS) is one of the most studied chemical reactions in the world. How H_2 and CO interact with a very well-known Fe/C surface will help to understand at an atomic level this synthesis. Although Fe is not the most active transition metal for FTS, the low price, the different products that can be obtained and the wide temperature range in which it can be used, from 200°C to 350°C, make it interesting for industry.

Thermal evaporation is used to evaporate a few monolayers of Fe and C on top of Cu(100), that will act as a support for the flat single crystal Fe/C catalyst. Deposition is performed in ultra-high vacuum conditions with a base pressure of $3x10^{-8}$ Pa and holding the sample at the desired temperature can help us to avoid interdiffusion, the threshold is less than 400K for the Fe/Cu(100) surface. The growth of Fe on Cu will depend on the deposition rate, base pressure during deposition, the temperature of the sample and how clean is the Cu substrate. Carbon can be evaporated using graphitic rods and also different carbon precursors such as acetylene or ethylene can be used.

Auger electron spectroscopy (AES) is an important analysis technique in this project. The chemical information that can be obtained with AES is vital in order to determine both concentration and chemical nature of the iron and iron carbide phases created. In addition to this, Low Energy Electron Diffraction (LEED) provides information about the structure of the Fe and FeC_x films and can also be used to determine whether adsorbates such as CO and H_{ad} form ordered overlayers on the model catalyst. Kelvin probe and temperature programmed desorption techniques will be used to study adsorption and desorption of the FTS reactants, CO and H_2, as well as elementary reactions steps that involve FTS intermediates and products, i.e. C_xH_y surface chemistry.

References:
[1] C.Egawa, E.McCash, R, Willis. Surf.Sci. **215**, L271-L278 (1989)
[2] C.J.Weststrate, P.Van Helden, J.W. Niemantsverdriet. Catal.Today, **275**,100-110(2016)
[3] H.Jenniches, M.Klaua, H.Hoche, J.Kirschner. Appl.Phys.Lett, **69**, 3339-3341(1996)
[4] W.Arnott, W.Allison. Physica B, **289**, 1-3(1989)