Comparison of CO adsorption and dissociation on flat, stepped and kinked Co surface

Devyani Sharma[1], Kees-Jan Weststrate[2]

[1]*Dutch Institute for Fundamental Energy Research, De Zaale 20, 5612 AJ Eindhoven, The Netherlands*

[2]*SynCat@DIFFER, Syngaschem BV, P.O. Box 6336, 5600 HH Eindhoven, The Netherlands*

D.sharma@differ.nl

The Co based catalyst used for the Fischer-Tropsch synthesis (FTS) reaction consists of nm-sized Co nanoparticles dispersed on a high surface area support. From a model of such a particle, shown in figure 1(a), it can be seen that both close packed as well as step and kink sites are exposed [2]. As CO is a reactant in FTS, it is of interest to study how it interacts with the various structural elements exposed by a nanoparticle surface.

The aim of the present work is to compare CO adsorption on flat Co (0001), stepped Co (10-19) and Co (10-120) and kinked Co (11-29) surface. The adsorption energy of CO at step sites, where the Co atoms have a lower coordination number than those on the close-packed terraces, is expected to be different than at the highly coordinated terrace sites on Co surface. Yet, the high temperature CO desorption peak [figure 1(b)] is found at the same temperature for all the surfaces under consideration, and the coordination number of Co atoms does not appear to play a role.

The low temperature CO desorption peaks are broader as well as shifted for the Co (11-29) surface compared to the Co (10-120) and Co (0001) surfaces. This is attributed to the small width of the close-packed terraces on the Co (11-29) surface, which is too small to accomodate the ordered structures that exist for high coverages on the flat Co (0001) terrace. The larger terrace width of the stepped Co (10-120) surface mimic the flat Co (0001) surface and consequently their CO desorption spectra look more similar.

For the stepped surface a small CO desorption peak is found around 600 K (figure 1(c), inset). This can be attributed to recombination of carbon and oxygen, formed by CO disproportionation at step sites. Interestingly such a peak is not observed for the kinked surface. Further investigations are required to better understand the reactivity for CO dissociation of kink sites.

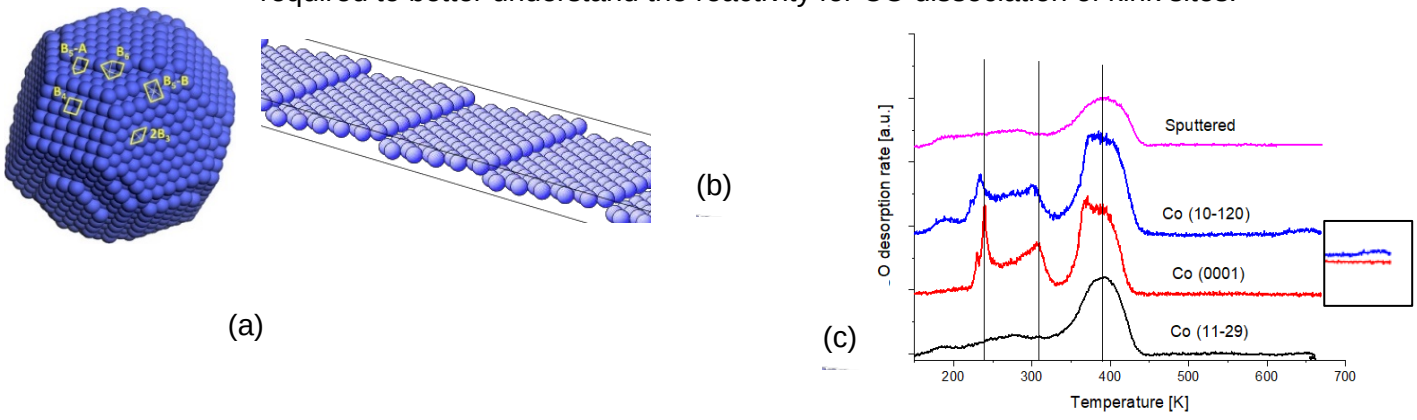

Figure 1: (a) Co particle model, adapted from ref. [2], showing the close-packed terraces, step sites and kink sites. (b) Co (11-29) surface adapted from surface explorer (c) CO TPD spectra comparing results on Co (0001), Co (11-29) and Co(10-120)

References:

[1] Weststrate, C. J., J. van de Loosdrecht, and J. W. Niemantsverdriet. *Journal of Catalysis* 342 (2016): 1-16

[2] van Helden, Pieter, Ionel M. Ciobîcă, and Roelof LJ Coetzer. *Catalysis Today* 261 (2016): 48-59.