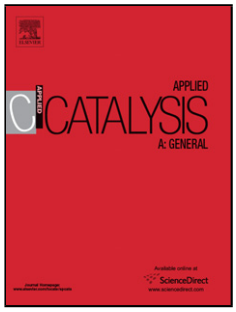

Title: Kinetic modelling of temperature-programmed reduction of cobalt oxide by hydrogen

Authors: Chao'en Li, Lisa Wong, Liangguang Tang, Nicola V.Y. Scarlett, Ken Chiang, Jim Patel, Nick Burke, Valerie Sage

PII: S0926-860X(17)30088-1
DOI: http://dx.doi.org/doi:10.1016/j.apcata.2017.02.022
Reference: APCATA 16158

To appear in: *Applied Catalysis A: General*

Received date: 30-11-2016
Revised date: 24-2-2017
Accepted date: 28-2-2017

Please cite this article as: Chao'en Li, Lisa Wong, Liangguang Tang, Nicola V.Y.Scarlett, Ken Chiang, Jim Patel, Nick Burke, Valerie Sage, Kinetic modelling of temperature-programmed reduction of cobalt oxide by hydrogen, Applied Catalysis A, General http://dx.doi.org/10.1016/j.apcata.2017.02.022

<AT>Kinetic modelling of temperature-programmed reduction of cobalt oxide by hydrogen

<AU>Chao'en Li[a], Lisa Wong[at], Liangguang Tang[a], Nicola V. Y. Scarlett[b], Ken Chiang[a§], Jim Patel[a], Nick Burke[a], Valerie Sage[c]* ##Email##Valerie.Sage@csiro.au##/Email##
<AU>
<AFF>[a]CSIRO Energy, 71 Normanby Road, Clayton North, VIC 3169, Australia
<AFF>[b]CSIRO Mineral Resources, Bayview Avenue, Clayton South, VIC 3168, Australia
<AFF>[c]CSIRO Energy, Australian Resources Research Centre, 26 Dick Perry Avenue, Kensington, WA 6151, Australia
<AFF>[t]Current address: Institute for Frontier Materials, Deakin University, 221 Burwood Highway, Burwood, VIC 3125, Australia
<AFF>[§]Current address: School of Engineering, RMIT University, Melbourne, VIC 3000, Australia

<PA>Tel.: +61 8 64368836; Mobile: +61 423970136; Fax: +61 8 64368555.

Highlights►

<ABS-Head><ABS-HEAD>Graphical abstract
<ABS-P>
<ABS-P><xps:span class="xps_Image">fx1</xps:span><ABS-HEAD> ► Highlights ► A 5-steps reduction mechanism for *Co_3O_4* was proposed; ► The promoter improved the reducibility of *Co_3O_4* while little on *CoO*; ► Reduction difficulties follow the order: Ru-Co-La/Al_2O_3 < Ru-Co/Al_2O_3 < Co/Al_2O_3; ► High crystallinity increases the difficulty of reducing Co_3O_4 instead of intermediates; ► The interaction between *CoO* and *Al_2O_3* to form *$CoAl_2O_4$* was modelled.

<ABS-HEAD>Abstract

<ABS-P>The reduction activities and mechanisms of cobalt-based catalysts are of great interest to industry and researchers, due to their applications in Fischer–Tropsch synthesis. Here, we investigated the reduction of alumina-supported cobalt catalysts by hydrogen using temperature-programmed reduction. We propose a five-step reduction mechanism that incorporates both amorphous and crystalline Co_3O_4, and includes the interaction between CoO and the Al_2O_3 support. Based on our proposed mechanism, we developed a kinetic model of the reduction process. The modelling results of catalysts promoted with ruthenium and lanthanum in contrast with un-promoted catalyst clearly show that the promoter improves reducibility of the catalyst. The effect of Co_3O_4 crystallinity was also investigated by the reduction of fresh in comparison of pre-oxidised catalyst. We conclude that high crystallinity significantly increases the difficulty of reducing Co_3O_4. The interaction between CoO and Al_2O_3 under reduction conditions to form $CoAl_2O_4$ was quantitatively simulated. The kinetic modelling confirms that the support plays an important role in catalyst reduction via the interaction between the catalyst and the support. Those kinetic modelling results are supported by in situ X-ray diffraction studies of the reduction process.

<KWD>Keywords:
Catalysis; Temperature-programmed reduction; Cobalt oxide; Kinetic modelling; Reduction mechanism; Fischer–Tropsch synthesis

<td:DefL>Nomenclature **list**
<xps:span class=deft>I_i </xps:span> <xps:span class=defd>TCD signal intensity (a.u.) at time I;</xps:span>