

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Atomistic Thermodynamic Approach for Determining Cu Catalyst Morphologies Under Reactive Water-Gas-Shift Conditions NILAY INOGLU, JOHN KITCHIN, Dept. of Chemical Engineering, Carnegie Mellon University — The water gas shift reactions (WGS) are widely used in several industrial processes and are catalyzed by Cu catalysts. In coal derived syngas, there are sulfur (S) impurities which can adsorb on the Cu surfaces and block the active sites of the catalyst and can result in catalyst deactivation. The sulfur adsorption will compete with other possible adsorbates such as CO, O, H and CO₂ making a quantitative estimate of the impact of sulfur on reactivity difficult. To determine the interactions between these possible adsorbates with Cu, the adsorption properties of these different adsorbates on low Miller index facets of Cu surfaces were studied in the limit where these surfaces are in thermodynamic equilibrium with the reactive environment. The effect of S adsorption on the surface electronic structure was significant and coverage dependent. In addition to a site-blocking deactivation mechanism, we found that sulfur modifies the surface electronic structure in a way that makes the Cu less reactive. Our results show that the adsorbates play a key role in defining the catalyst morphologies. We conclude that the presence of sulfur and other reactive adsorbates can impact the reactivity of the catalysts through several mechanisms including site-blocking, surface electronic structure modification and changes in the distribution and types of reactive sites through catalyst morphology changes.

Nilay Inoglu
Dept. of Chemical Engineering, Carnegie Mellon University

Date submitted: 21 Nov 2008

Electronic form version 1.4