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Nanoparticle Interfaces Studied Using Environmental TEM and Atomic Scale Modelling

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Motivation and background

Supported heterogeneous catalysts play an essential role in areas such as automotive exhaust abatement, energy storage/conversion and sustainable production of chemicals. In order to gain insight into properties such as activity and stability of these materials, catalysts must be studied \textit{in situ} in reactive environments. Only a few experimental techniques allow for investigation of the materials at a local scale with atomic resolution while exposing samples to gases and elevated temperatures. Recent advances in high-resolution environmental transmission electron microscopy (ETEM) have shown that the atomic configuration at surfaces and interfaces of a metal nanoparticle is a function of its surroundings [1]. Similarly, the dynamics and hence stability of the catalyst are important parameters which can be studied using \textit{in situ} microscopy [2].

ETEM experiments

In order to study the influence of the environment on catalytic nanoparticles, model systems consisting of Au/CeO\textsubscript{2}, Pt/CeO\textsubscript{2}, Au/TiO\textsubscript{2} and Pt/TiO\textsubscript{2} were prepared using a physical method (sputter coating). For the preliminary \textit{in situ} experiments low gas pressures at room temperature were used.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{ETEM_experiments.png}
\caption{ETEM experiments}
\end{figure}

1) Sputter coat prepared Au/TiO\textsubscript{2} exposed to 0.45 mbar CO dose rate: 4.27E+4 e/Å\textsuperscript{2}.
2) FFT of Au particle and TiO\textsubscript{2} respectively, Au(1-11)/(TiO\textsubscript{2} (1-10).
3) Snap shots from an image sequence, arrows indicate the three top most layers of the particle.
4) The number of atomic columns in each layer of the particle as seen in image 3), the trend indicates that the dynamics is a fluctuating phenomenon.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Modelling_support_interfaces.png}
\caption{Modelling support interfaces}
\end{figure}

Precise information of what happens at the support interface is not directly available from experiment. We are developing theoretical models specifically for metal/oxide interfaces relevant for catalytic systems. Three qualitatively different examples are shown below.

Comparison between a free Pt nanoparticle and a similar particle supported on anatase TiO\textsubscript{2}. The small lattice mismatch of 3.4 % modifies the overall strain distribution.

Cu nanoparticle supported on alumina. The strain distribution of the bottom atomic layer of the particle reveals a dislocation network at the interface.

Pt nanoparticle supported on cubic ZrO\textsubscript{2}. The particle is unable to adapt to the large lattice mismatch of 24 %, leading to a disorganized strain distribution.

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References

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