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Q: The difference of theoretical and experimental patterns is rather high, why?

The difference between the experimental and theoretical patterns is large in the case of the Cu and Pd EXAFS because only the first nearest neighbour shell is fit, that only the atoms within 3 Å of the absorber. In contrast, the Au EXAFS is fit up to 6 Å and so the theoretical and experimental patterns is much less. The signal to noise ratio for Au is very large due to the amount of Au present, and therefore the data quality is very good and more information can be extracted from the EXAFS. In the case of the Cu and Pd, the amount is much lower as only a small layer/clusters on the surface is present and therefore the signal to noise ratio is much lower. As a result only the first nearest neighbour shell can be fit as beyond that the data quality is not good enough to extract structural information.

A secondary reason, although less visually apparent, is that the theory typically used to fit the EXAFS assumes an even distribution of bond lengths that have Gaussian disorder. This is not true in the case of nanoparticles as the atoms on the surface of the particle will be contracted towards the core to an extent that creates a splitting in the bond length distribution. The surface atoms will also have a different degree of freedom compared with those in the core of the particle. Both of these reasons mean the theoretical spectra will not quite match with the experimental spectra however the results of this are more apparent in the fitted parameters than in the visual fit. More information on this effect can be found in the following reference S. W. T. Price, N. Zonias, C.-K. Skylaris, T. I. Hyde, B. Ravel, and A. E. Russell 2012, Phys. Rev. B 85, 075439.

Q: What was the technology of underpotential deposition?

Underpotential deposition occurs at a potential positive to the bulk deposition potential and, on single crystal surfaces, reliably forms a monolayer of the deposited metal (Brankovic, S. R.; Wang, J. X.; Adzic, R. R. Surface Science 2001, 474, L173.). Firstly, the prepared nanoparticles were loaded on carbon, mixed into an ink, painted onto carbon paper, and hot-pressed to form an electrode. The electrode was hydrated and placed within the in-situ cell and a solution of 2mM $CuSO_4$ in 0.5 M H_2SO_4 pumped through. The cell was connected to a potentiostat and the potential gradually moved to the region of interest. Once at the region, e.g. upd onset, the current was monitored until it reached a steady state. At this point the EXAFS was measured (Price et al. JACS 133, 19448-19458, (2011)).

Q: What was X axis at the plots with numerous maxima?

The different plots shown on slide 5 used for EXAFS are: a) mu(E) or normalised mu(E) vs E, units eV b) chi(k) vs k, units Å-1 and c) Fourier transform of chi(k) vs. R, units Å.