Structure Determination of Noble Metal Clusters by Trapped Ion Electron Diffraction

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The structures of noble metal cluster ions have been studied by the recently developed technique of trapped ion electron diffraction (TIED) [1]. In brief, cluster ions are generated by a magnetron sputter source and injected into a quadrupole ion trap. After mass selection and thermalization, the trapped ions are irradiated with a 40 keV electron beam. The resulting diffraction pattern is integrated with a CCD detector. The assignment of the cluster structures is done via a comparison of the experimental and simulated scattering function, calculated from density functional theory structure calculations.
The structures of mass selected silver cluster cations Ag_{19}^+, Ag_{38}^+, Ag_{55}^+, Ag_{59}^+, Ag_{75}^+ and Ag_{79}^+ have been investigated [2]. The resulting experimental data are best described by structures based on the icosahedral motif, while closed packed structures could be ruled out.

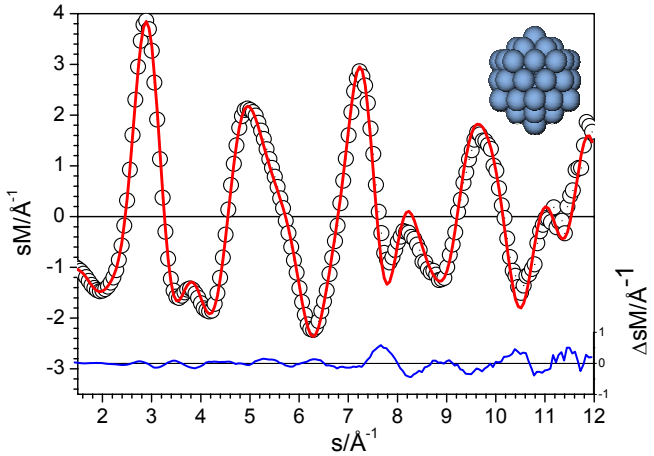

Figure 1: Comparison of experimental (open circles) and model (line) reduced molecular diffraction functions sM for the icosahedral isomer of Ag_{55}^+ (inset) at 100K. The lower trace shows the residual.

Additionally, we present a comparison of the structures of $Cu_{20}^{+/-}$, $Ag_{20}^{+/-}$ and $Au_{20}^{+/-}$. Our findings show unambiguously that the structure of Au_{20}^- is given by a tetrahedron in agreement with the results of L.S. Wang et al. [3]. In contrast, structures of Ag_{20}^+ and $Cu_{20}^{+/-}$ based on the icosahedral motif agree best with the experimental data. Small structural differences between the charge states are observed. The possibilities and limitations of the TIED method are discussed.

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