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 $\text{Ag}_{19}^+$, $\text{Ag}_{38}^+$, $\text{Ag}_{55}^+$, $\text{Ag}_{59}^+$, $\text{Ag}_{75}^+$ and $\text{Ag}_{79}^+$ 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 $\text{Ag}_{55}^+$ (inset) at 100K. The lower trace shows the residual.](image)

Additionally, we present a comparison of the structures of $\text{Cu}_{20}^{+/-}$, $\text{Ag}_{20}^{+/-}$ and $\text{Au}_{20}^{+/-}$. Our findings show unambiguously that the structure of $\text{Au}_{20}^-$ is given by a tetrahedron in agreement with the results of L.S. Wang et al. [3]. In contrast, structures of $\text{Ag}_{20}^{+}$ and $\text{Cu}_{20}^{+/-}$ 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.