Experimental and Theoretical Determination of Low Electron Energy Loss Spectra of Ag and Ru

D. S. Su¹, W.-D. Schöne¹, C. Hébert²

¹ Fritz-Haber-Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany
² Institute for Solid State Physics, Technical University of Vienna, Wiedner Hauptstrasse 8-10, A-1040 Wien, Austria

Very complex materials and highly correlated electronic systems in reduced dimensions become currently one of the main investigation topics in condensed matter physics. However, understanding the behavior of these new and exciting materials requires a detailed understanding of electronic correlation. Comparatively simple systems, e.g., noble metals in the crystalline phase, have therefore gained renewed interest. We present in this work the results of the dynamical electronic response of Ag and Ru determined by EELS-experiment and by ab-initio calculations. The comparison of the theoretical calculation with the experimental data allow the analysis of the many-body and crystal local-field effects. The calculations are carried out in the framework of the Random Phase Approximation (RPA) and the time-dependent local density approximation (TDLDA), which also accounts for vertex corrections. Experiments were performed on a Philips CM 200 FEG TEM and on a TG 200 FEG TEM, operated at 200 kV. A GATAN imaging filter was used to record the EEL-spectra. The Ag and Ru single crystals were prepared by polishing and ion-milling until electron transparency. In diffraction mode, the pattern is moved over the entrance aperture of the energy filter to choose the demanded \( q \) values. The recording time varies from 10 to 60 s according to the chosen momentum transfer.

![Graph](image)

**FIG. 1.** left: Experimental and theoretical spectrum of Ag; right: Influence of crystal local-field effects on the density-response function.

Both experiment and theoretical calculations show a \( q \)-dependent dynamic response in single crystal Ag and Ru. The results for \( q = (\frac{1}{2}, \frac{1}{2}, 0) \) of Ag are displayed in Fig. 1 (left). While the spectrum feature between 20 to 40 eV are found in both results, the matching for energy region less than 20 eV is not satisfying. The imaginary part of the density-response function of the \( G'=0 \) is also presented in Fig. 1 (right). Details about the electronic response at other \( q \) values and in Ru will be presented.

Reference

[1] This research was initiated and motivated by Dr. Walter Ekardt.