ROBL-CRG	**Experiment title:** **Structural and magnetic properties of ternary uranates at low temperatures. Mixed valence effects in NaV_2O_5 single crystals.**	**Experiment number**: 20-01-651
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Report:

We investigated the charge fluctuations and mixed valence effects in NaV_2O_5 single crystals. The measurements of the XANES and EXAFS spectra of NaV_2O_5 and $N_{0.95}V_2O_5$ are performed at the room temperature and at 15 K. The results are compared with calculations based on self-consistent real space full multiple scattering analysis. A comparison between experimental and theoretical V K edge XANES of NaV2O5 crystals is presented in Figure 1. The lowest energy structure is the peak A with a low energy shoulder A1 is found to be a characteristic feature for all mixed V4.5 +. In the higher energy region of the XANES, we observed the shoulders B and C, which are h are s indicators for the perfect perovskite structure. The D and E doublet appears as a consequence of V-O layered structure along the c-axis.

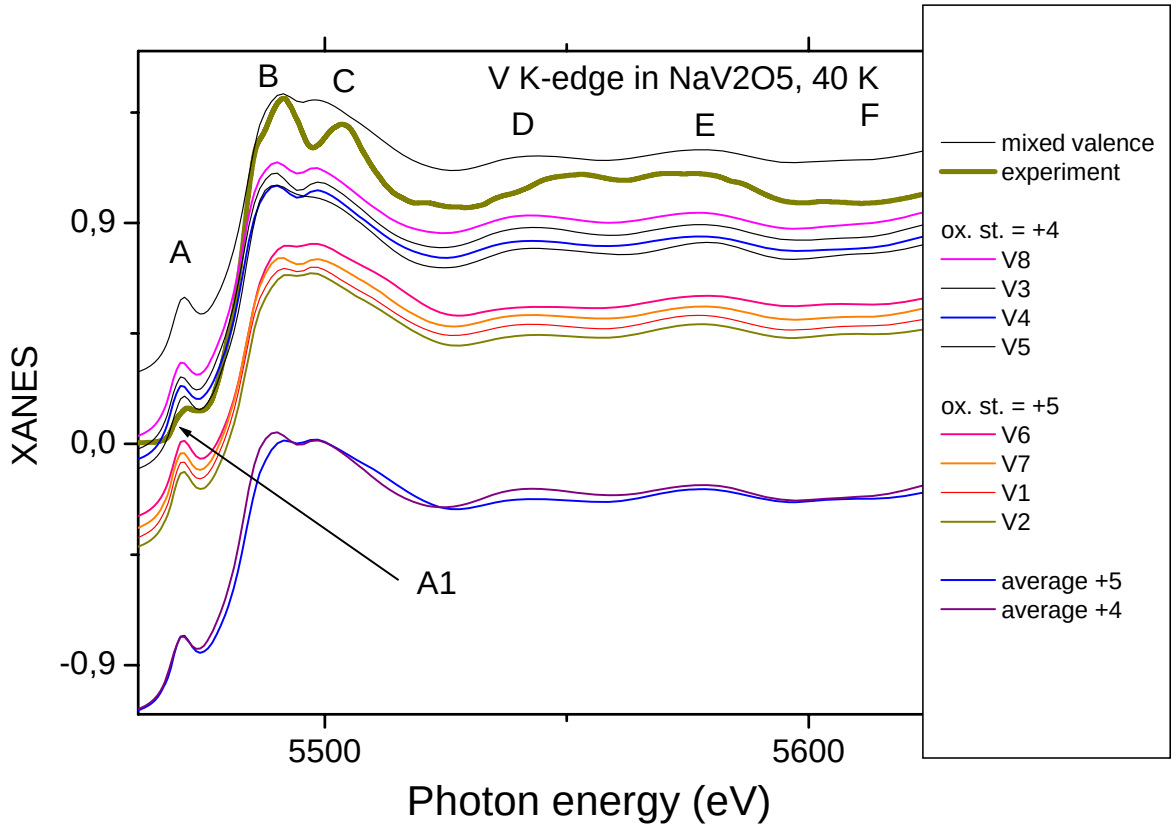

Figure 1. Comparison of the experimental V K edge XANES in NaV_2O_5 single crystals with the theoretical spectra.

The calculated spectra exhibit an oversmoothed white line feature as compared to experimental spectra and the lack of A1 feature. This seems to be a common fault of calculations in Hedin Lundquist potentials, and indicates that interaction which describes the electron correlations within V-O-V rungs needs to be included in the model.