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Report:

The proposal was addressed to study of local structure of colour/impurity centres in synthetic and natural emeralds by x-ray absorption spectroscopy. During the allocated beamtime we measured several samples of emeralds coming from different sources. The natural samples were from Sandowana, Zambia and Brazil while the synthetic samples were grown by flux and hydrothermal methods. In addition we also measured natural Beryl samples to compare with the emerald samples. The work was focused on absorption measurements at K-edges of Fe, Cr and V elements. However, we measured Fe K-edge spectra on the natural Beryl as this sample was free from other impurities such as Cr and V.

The monochromator crystal was Si(111) with sagital focusing while the detector system was a multi-element fluorescence yield (FY) solid state detector. The FY detection was one of the necessary requirements of the experiment as this allowed us to extract partial cross section only due to the required transition element for a particular measurement. This approach allowed us to measure the absorption spectra with high signal to noise ratio in the dilute systems. All the measurements were performed at room temperature.

We used single crystal samples of all these emerald samples and measured absorption spectra at all the above edges. However, We had to face a number of glitches in the spectra due to the diffraction peaks of the Beryl system. Due to complexity of the structure, it was hard to get rid of all the diffraction peaks and hence we were obliged to measure absorption spectra upto a limited k-range. In such a situation our attention was focused on the near edge (XANES) part of the spectra. The data are being analysed and the results will be reported elsewhere (in the final experimental report).

During the experimental run, we could also took time to study the local structure of Cr in Ruby samples. The natural Ruby samples measured have different origin. For comparison, we have also measured synthetic samples of Ruby. All these measurements were focused at the Cr K-edge XANES. The spectra were first measured on single crystal samples but unwanted polarisation effect in the XANES spectra forced us to crush the Ruby samples. This allowed us to make a systematic spectral differences in the XANES spectra on Rubies coming from different origin.

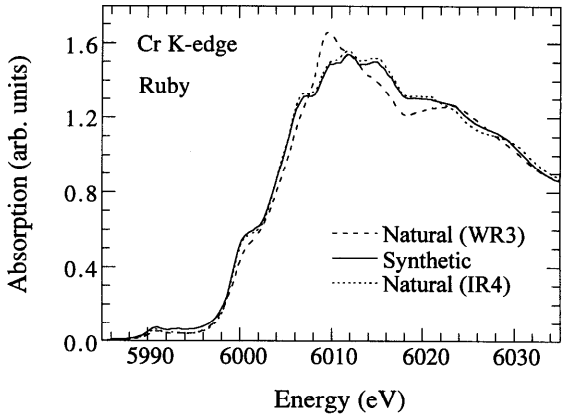

Fig. 1. Normalized Cr K-edge absorption spectra on different Rubies.

We have shown a representative comparison between the Cr K-edge XANES spectra measured on different Rubies. For the purpose, a XANES spectrum on synthetic sample has been compared with samples coming from natural sources. This preliminary analysis of the data clearly show that the local structure of Cr in these samples is quite different. The present study suggests that a careful work is needed on several samples to establish the differences in the local structure of Cr impurity in the studied system. A systematic EXAFS study is planned for the near future to quantify the local structural differences. A detailed analysis of the data is still to be done.