ESRF	**Experiment title:** High resolution electron density study of Al_2O_3	**Experiment number:** CH-241
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Report:

The experiment served three purposes. The first was to test the newly installed SIEMENS CCD system for accurate electron density studies. The second was to obtain a high quality data set on Al_2O_3. The third was to perform multiple-wavelength measurements in order to get an experimental assessment of the extinction effects, which are known to be large for this compound.

The SIEMENS detector proofed to be suitable for doing high resolution diffraction work, even at energies as high as 58 keV. Optimum use of the data processing software was relatively straightforward. A great advantage of this detector over the previously used image intensifier/CCD system is the fact that no re-calibration is needed when the energy or set-up is changed.

A full data-set was collected at 58 keV and 120 K. A completeness of 100 % with a redundancy of 7 was obtained up to a resolution of $sin\Theta/\lambda = 1.25\mathring{A}^{-1}$, by collecting data-sets at different crystal settings. The data were scaled and merged using a modified version of, SORTAV, giving an overall R_{merge} of 5.5 % and 462 unique reflections. The data were then refined against a multipole model using MOLLY, with the standard multipoles at the atoms. An excellent fit was obtained giving a refined R-factor (on F) of 1.36 %, with a goodness-of-fit of 1.34. Figure 1 gives the static deformation density in the AI-O plane. The quality of the data can be seen by the fact that in the Al-O(l) bond the density is higher than in the Al-O(2) bond. This agrees with the fact that the Al-O(l) bond is shorter than the Al-O(2) bond. Also the agreement with theoretical data is good. These results are submitted to Acta Cryst. B.

Subsequently, data-sets were measured at 5 different energies: 15, 27, 39, 50 and 58 keV. Using the results of the 58 keV data-set as starting point, the data were refined against a multipole model, including extinction. (Becker/Coppens formalism).

The data were also analyzed by a model-free approach, in order to estimate the extinction. Figure 2 gives the extinction parameters for the 116 and 113 reflections as function of wavelength. The solid lines correspond to the Becker/Coppens model, and the dashed lines to the model-free estimate. The results of the model-free approach are normalized to the shortest wavelength. The results indicate a possible underestimate of the extinction at the highest energy for the Becker/Coppens model. The data is currently further processed, and the full results will be published in a second paper soon.

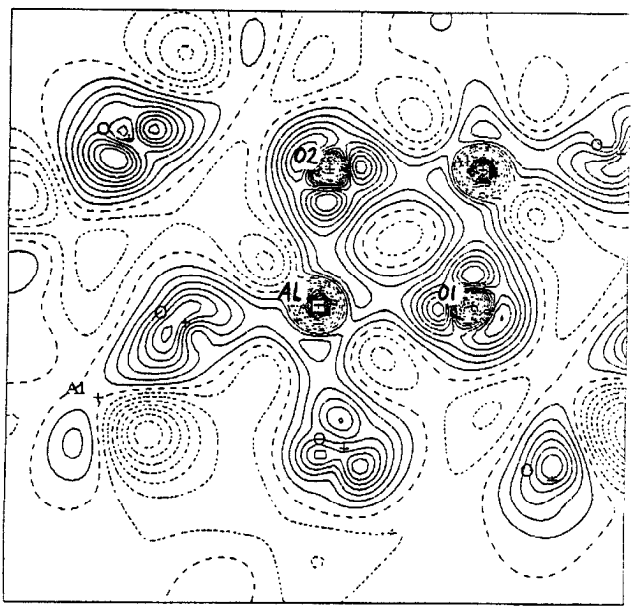

Fig. 1

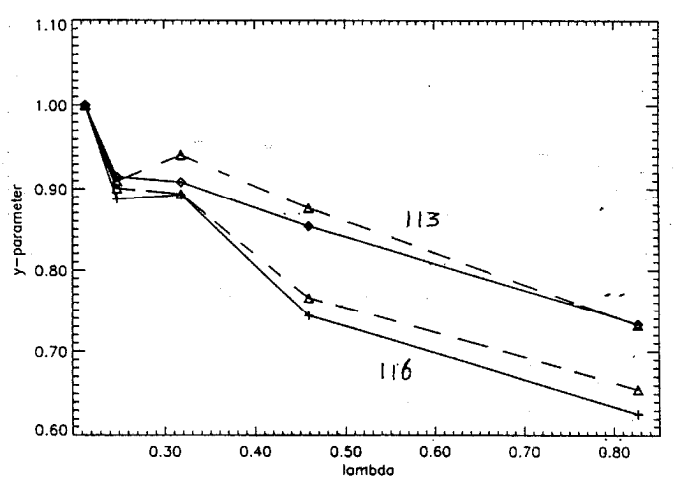

Fig. 2