ESRF	**Experiment title:** ANOMALOUS DIFFUSE SCATTERING IN YTTRIA-STABILIZED ZIRCONIAS	**Experiment number**:HS1702
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Report

Pure zirconia (ZrO_2) presents three allotropic structures: cubic at high temperature, down to 2369°C, tetragonal between this temperature and 1114°C, and monoclinic below 1114°C. As these solid state transformations rise difficulties for technical applications, they are suppressed by stabilization, i.e. doping with other oxides. This doping extends the stability domain of the cubic phase. The most frequent dopant for zirconia is yttria (Y_2O_3) : the material is then termed "yttria stabilized zirconia" (YSZ).

We have started a numerical simulation program, using Molecular Dynamics (MD) and Monte-Carlo (MC), in order to study the thermal conductivity (TC) of YSZ. The TC is expected to be very sensitive to the state of order of the system, in particular to the short range order. For conventional X-rays as for neutrons, the structure factors of Y and Zr are very similar. In these conditions only correlations between undistinguishable Y and Zr and Oxygen can be accessed trough Diffuse Scattering (DS). The use of anomalous dispersion gives access to the correlations between Y and Zr.

In order to collect informations about the Y-Zr correlations, we have measured the Anomalous Diffuse Scartering (ADS) of X-Rays on one of the single crystal samples that were measured by neutrons. The incident energy was 16500 and 17000 eV, i.e 538 and 38 eV below the Y threshold (17038eV). We have also used 17963 eV, 35eV lower than the Zr threshold

(17998eV). Contour plots of the intensity distributions in the 110 plane are shown on the figure. They correspond to 17998 (left) and 17000 eV (right, common scale): though the complete data reduction is not yet performed, there are clear changes of shape of the contour plots.