



	Experiment title: COMPENSATION MECHANISMS IN Cl DOPED POLYCRYSTALLINE CdTe: THE STRUCTURE AND THE LOCALIZATION OF THE BETA ACCEPTOR COMPLEX	Experiment number: MA - 520
Beamline: ID21	Date of experiment: from: 25 June 2008 to: 30 June 2008	Date of report: September 2008 <i>Received at ESRF:</i>
Shifts: 15	Local contact(s): Dr. Marine COTTE	
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Report:

Our experiment was in fact technically un-feasible because of the too low transmission (#10-15%) of the Fresnel zone plate used to generate a microbeam. Therefore, we lack photon flux and we were not able to record μ XAS spectra at Cl edge at various localization of the samples, namely at grain boundaries, inside grain or twin boundaries aso. Use of a KB system - which offers much better transmission - may make this experiment technically feasible on ID21.

As microbeam provides us with a too low flux, we were forced to use the 100 μ m pinhole-defined beam on our samples. ID21 staff then successfully implemented the recording of EXAFS spectra on a large energy range extending 400eV after edge. With this large beam, we illuminated our 2 study sample E1415 and E1419, the first being rich in well-known A-center while the second is rich is the Beta-acceptor complex.

The enormous drawback here is that using a large beam prevents us from local Cl concentration reinforcement. Therefore, we dealt here with Cl atomic concentration of 10^{17}cm^{-3} with an incoming photon flux of 5.10^{10} Photons/s. Consequently, the signal-to-noise ration allow only recording of medium quality XAS spectra, and requires a 24 hours duration. Recorded spectra are presented on figure 1.

As can be seen, the baseline of recorded spectra stays flat until 2950eV where it clearly rises up. This comes from the presence of a - completely unawaited - very intense RAMAN spectra. During an energy scan, this raman spectra shifts towards higher energy with incoming energy and around 2950eV, it enters the ROI defined in the detector to select the fluorescence energy of Cl, thus making the baseline rise up. Complete fluorescence spectra as a function of energy are presented in figure 2.

Comparison between extracted EXAFS oscillations are presented figure 3. The medium quality of recorded data and the presence of the raman contribution clearly limits the useful k-range and leads to a noisy Fourier transform as shown on figure 4. Despite a clear difference is visible between the E1415 and E1419 k spectra especially at small k, EXAFS fitting using the feffit package did not lead to any clear picture of what happens to the second shell around

Cl. Indeed, the Chi(R) figure does show a difference in the second shell around 4Å but it was too noisy to realize any significant fit. This is really a pity since the beta acceptor complex lies specifically in the second shell around Cl.

We were still able to compare first shells between E1415 and E1419. In both case, we get Cd as first neighbours with -6eV as E_0 , almost identical Debye-Waller factor $\sigma^2=25.5 \cdot 10^{-3} \text{Å}^2$ (which is awaited since Cl localisation is mainly at grain boundaries), same distance Cl-Cd = $2.45 \text{Å} \pm 0.02 \text{Å}$ (12.5% contraction). Main difference is that in the case of E1419, we get an average of 3Cd while 2.5 for the E1415. We were not able to go any further in the EXAFS interpretation.

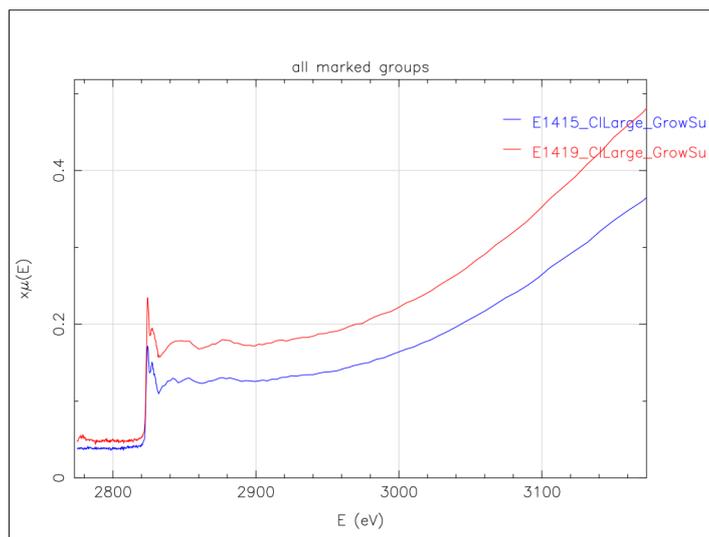


Figure 1: recorded XAS spectra

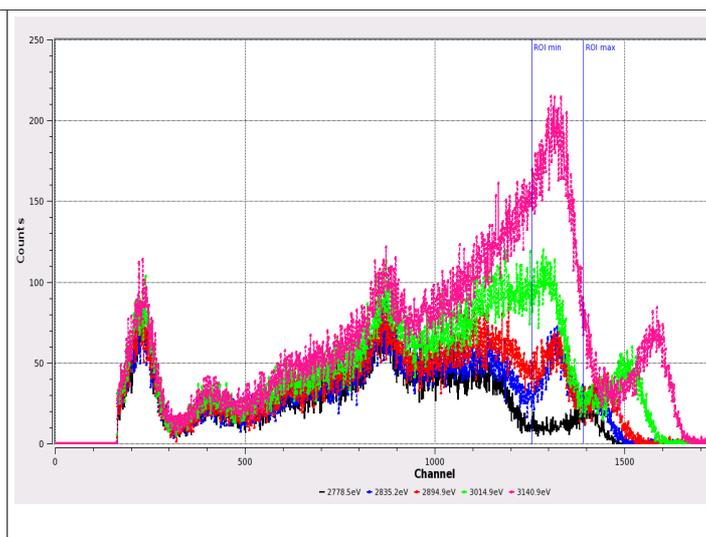


Figure 2: fluorescence spectra recorded by the energy-resolved detector as a function of incoming energy. ROI min and ROI max mark the fluorescence energy band of Cl. The raman contribution is clearly visible as well as its shift toward energy with incoming energy.

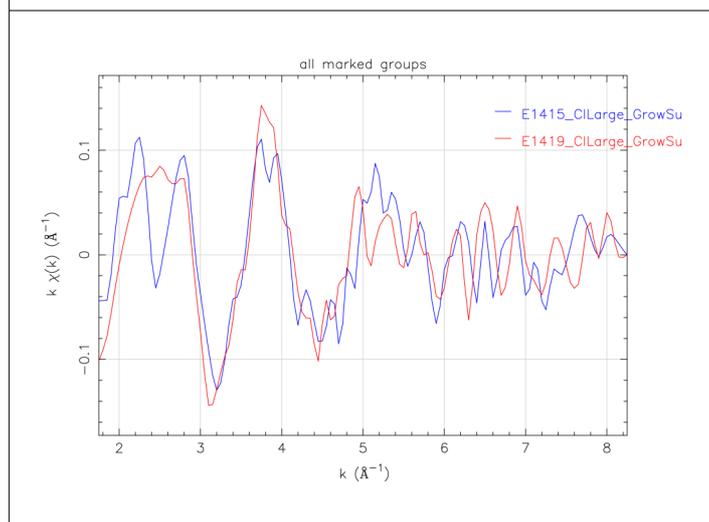


Figure 3: comparison between E1415 and E1419 exafs oscillations.

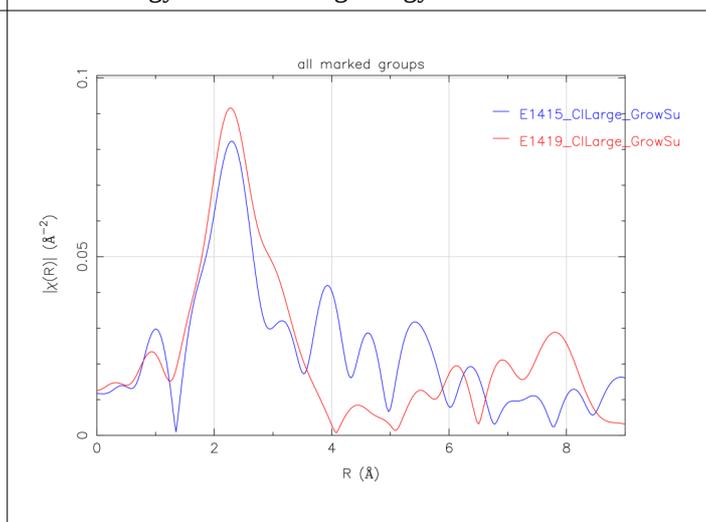


Figure 4: comparison between E1415 and E1419 Fourier transformed exafs oscillations.