



	<b>Experiment title:</b> <u>Search for an electric dipole moment in non-centrosymmetric metallic CeCoGe<sub>3</sub> crystal</u>	<b>Experiment number:</b> <b>HC-2083</b>
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## Report

### Scientific Background

The main goal of this experiment was to record natural circular dichroism in resonant x-ray diffraction in metallic CeCoGe<sub>3</sub> single crystal and to show that this technique could be used to detect the existence of dipole moment in metals and to measure its value in an element selective manner. The problem whether metals could exhibit ferroelectricity has been a puzzle since discovery of this ordering in solids [1]. Indeed in metals static internal electric fields (if exist) are screened by conduction electrons and as consequence no external field could be detected. Nevertheless recently ferroelectric-like structural transition was reported in a metallic LiOsO<sub>3</sub> below structural transition from centrosymmetric to non-centrosymmetric space group [2]. In a metallic crystal CeCoGe<sub>3</sub> the symmetry group allows the antisymmetric third-rank tensor due to E1E2 interference term which contains an irreducible part that transforms as a polar vector [3]. For this purpose we intended to measure the h00 forbidden reflections with circular polarization aiming to study the asymmetry ratio  $\sim [I_L(hkl) - I_R(hkl)] / [I_L(hkl) + I_R(hkl)]$  on the X-rays energy in the vicinity of absorption edges of Ce, Co and Ge.

### Experimental details

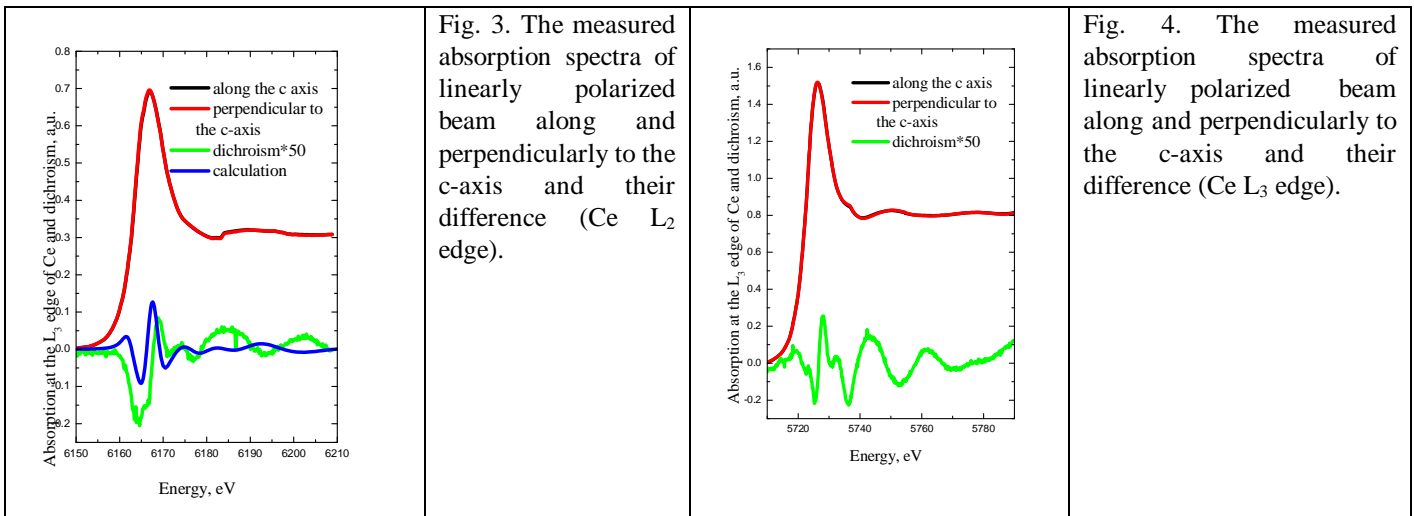
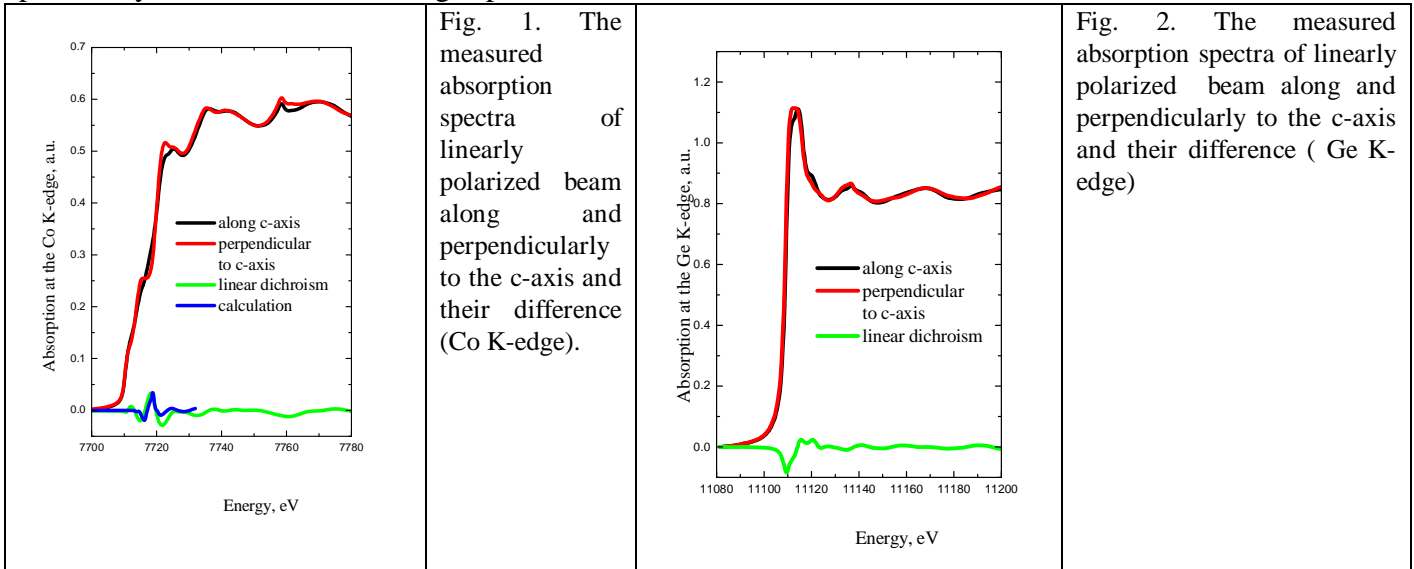
CeCoGe<sub>3</sub> single crystal is available for experimental study. But unfortunately, the miscut of the surface did not allow us to find an experimental configuration at ID12 beamline that would allow us to record the forbidden (100) reflection. So, the X-ray linear dichroism was measured at the absorption edges: K-edges of Co (7709 eV) and Ge (11103 eV) and Ce L<sub>1</sub> (6548 eV), L<sub>2</sub> (6164 eV), L<sub>3</sub>(5723 eV). X-ray absorption spectra were recorded at room temperature using total X-ray fluorescence yield detection mode along and perpendicularly to the four-fold axis. For these measurements we have used circularly polarized x-rays emitted by an Apple-II type undulator. After monochromatization by Si<111> double crystal monochromator the circular polarization of x-ray beam was converted by a diamond quarter wave plate into linear one, either vertical or horizontal. The polarization was flipped at every point of the energy scans.

### Results

The space group of CeCoGe<sub>3</sub> I4mm does not allow to observe X-ray natural dichroism because the corresponding third rank tensor does not contain a pseudoscalar part arising from electric dipole - electric quadrupole (E1.E2) interference term. Nevertheless, this symmetry allows to observe the X-ray linear

natural dichroism near the absorption edges of all elements. This dichroism occurs because of the valence electrons levels splitting by crystal field.

The measured absorption spectra of the polarized beam with two orthogonal linear polarizations are shown in the figures 1-4. We can see that the linear dichroism signal (the difference of the absorption corresponding to two orthogonal polarizations) is much more strong at the Co and Ge K-edges than at the Ce  $L_{2,3}$ -edges. The L-edges corresponds to the p to d transitions while the K-edges correspond to the  $s \rightarrow p$  transitions. Possibly the d-states of Ce are more localized and less splitted than the p-states of Co and Ge. Also we can see that the absorption spectra of Ge and Ce contains the strong 'white line' while it is practically absent in the Co K-edge spectrum.



First FDMNES [4] simulations of the linear dichroism in  $CeCoGe_3$  have shown that absorption edges and linear dichroism are well reproduced for the Co K-edge, but not so good for the Ge and Ce edges. Clearly more sophisticated calculations are needed and they are in progress.

**References**

[1] Anderson P.W., Blount E.I. Phys. Rev. Lett. 14, 217-219 (1965).  
 [2] Yanfeng Guo, Xia Wang, Andrew J. Princep, et al. Nature Materials. 12,1024-1027(2013).  
 [3] Jerphagnon J., Chemla D. J. Chem. Phys.65 1522 (1976).  
 [4] [www-cristallo.polycnrs-gre.fr/Themes-de-recherche/Simul/](http://www-cristallo.polycnrs-gre.fr/Themes-de-recherche/Simul/)

**Report Summary**

X-ray absorption of the linear polarized along and perpendicular to the c axis beam was measured in  $CeCoGe_3$  at the Co and Ge K-edges and at the  $L_{2,3}$  edges of Ce. The measurements have shown that the linear dichroism is more pronounced at the Co and Ge K-edges than at the Ce L edges. The calculations which describe the details of polarized absorption spectra and the dichroism spectra are in progress.

