Contribution ID: **40** Type: **Invited oral contribution**

Combined, Modulation Enhanced X-ray Powder Diffraction and Raman Spectroscopic Study of Structural Transitions in the Spin Crossover Material [Fe(Htrz)(trz)](BF)

Wednesday, 4 July 2012 16:20 (30 minutes)

The structure of [Fe(Htrz)2(trz)]BF4 (1, Htrz)1,2,4-4-H-triazole, trz) 1,2,4-triazolate) at the low-spin (LS) and high-spin (HS) states and structural transitions between the two states were investigated by in situ high- resolution synchrotron X-ray powder diffraction (XRPD) combined with Raman spectroscopy using a modulation-enhanced technique. The differences in the behavior of the spin transition observed by XRPD and Raman spectroscopy were explained by the local sensitivity of the two different techniques
and also by the spatial propagation of spin crossover phase transition within the crystallite and the body of the grain. Moreover, we demonstrated that the two-dimensional correlation analyses facilitate (i) understanding the data obtained by combined techniques, (ii) clarifying correlation between the signals gained by the different probes, and (iii) extracting information on temporal evolution of transformation processes. The stimulus have been applied periodically to esploit modulation enanched [ME]techniques in both spectroscopy, i.e. MES [1], and diffraction, i.e. MED [2]. The power and potential of MED as well as the combined two powerful modulation-enhanced techniques, MES-MED, will be shown taking spin-crossover materials as example [3].
[1] Urakawa, A. et al. Chem. Eng. Sci. 2008, 63 (20), 4902
[2] D. Chernyshov et al. Acta Crystallographica Section A 2011, A67, 327
[3] A. Urakawa et al.„ 2011, J. Phys. Chem. C, 115 (4), 1323

Primary author: Dr MILANESIO, Marco Milanesio (Universita' Piemonte Orientale)

Co-authors: Dr LUCA, Palin (Universita' Piemonte Orientale); Dr ATSUSHI, Urakawa (iciq); Dr WOUTER, van Beek (SNBL)

Presenter: Dr MILANESIO, Marco Milanesio (Universita' Piemonte Orientale)

Session Classification: Materials & Time Resolution Session

Track Classification: Materials / Nanomaterials