Charge Density Study of Photo-Excited State in Spin Crossover Complex

Kenichi Kato[a,b], Yutaka Moritomo[a,b,c], Masaki Takata[a,b], Akio Nakamoto[d], Norimichi Kojima[d], [a]*JASRI/SPring-8.* [b]*CREST/JST.* [c]*Department of Applied Physics, Nagoya University.* [d]*Graduate School of Arts and Sciences, University of Tokyo*, *Japan*. E-mail: katok@spring8.or.jp

The spin crossover complexes are widely recognized for the temperature and photo-induced transitons from low-spin (LS: S=0) to high-spin (HS: S=2) state of the Fe^{2+} io1ns. By the photo-excitation at low temperature the HS state is trapped even after the photo-irradiation. This phenomenon is called Light Induced Exited Spin State Trapping (LIESST). Here we have found the photo-excited state in $[Fe(ptz)_6](BF_4)_2$ [1] and $Fe(phen)_2(NCS)_2$, at 92K. At this temperature the LIESST phenomenon is not observed. The experimental and analytical methods used are as follows.

The powder diffraction data of the complexes were measured at 92K under 532nm CW laser irradiation by using Large Debye-Scherrer Camera installed at BL02B2, SPring-8. An imaging plate was used as a detector to collect whole powder patterns simultaneously. The N_2 gas flow type system was combined with the laser system for the low-temperature measurements. As a result, the volume ratio of the photo-excited phase reached to approximately 90 %. The charge density obtained by using the MEM/Rietveld method revealed the distinguished difference between the photo and temperature-induced HS state in the Fe-N bonding nature. In the talk, the detail including the LIESST phase will be presented.

[1] Moritomo Y., et al., *J. Phys. Soc. Jpn.,* 2002, **71**, 2609.

Keywords: photo-excited structure, spin crossover complex, charge density study