MS24 O1

Out of equilibrium charge density studies of light-induced metastable states Sébastien Pillet[a], Vincent Legrand[b], Mohamed Souhassou[a] & Claude Lecomte[a]. [a] Laboratoire de Cristallographie et Modélisation des Matériaux Minéraux et Biologiques, Nancy-Université, 54506 Vandoeuvre-les-Nancy, France. [b] Institut Laue Langevin, 6 rue Jules Horowitz, 38042 Grenoble, France. E-mail: sebastien.pillet@lcm3b.uhp-nancy.fr

Keywords: electron density studies, metastable materials, photochemistry

The experimental electron density analysis is becoming a very mature field of research with outstanding applications in many areas of solid state physics and chemistry. This approach has allowed gaining new insights on bonding interactions in ground state systems often from joined experimental and theoretical methods. The extension of this technique to out of equilibrium systems is very promising and might surely lead to a better fundamental understanding of dynamic processes in solids such as phase transition or chemical reactivity [1]. Steady-state and time resolved x-ray diffraction techniques under external perturbation, like electric field [2], pressure or optical excitation [3], are more and more developed, mainly for structural purposes. We have shown that under appropriate and well controlled experimental conditions, accurate electron density distribution of metastable states can be derived [4]. State of the art in light-induced high resolution x-ray diffraction experiments and charge density analysis of molecular metastable states will be presented. Applications will cover light-induced phase transitions in Fe(II) spin-crossover complexes and solid state chemical reactivity.

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MS24 O2

Spin density and non collinear magnetization in anisotropic materials Arsen Gukasov. *Laboratoire Léon Brillouin (CEA-CNRS),Centre d'Etudes de Saclay,91191, Gif sur Yvette, France.* E-mail: arsen.goukassov @cea.fr

Keywords: spin density, polarized neutrons diffraction, magnetic anisotropy

Polarized neutron diffraction (PND) is an extremely powerful tool to provide information about the spin density distribution in magnetic materials. In the PND spin density studies the moment induced on the atoms by an external magnetic field is assumed to be collinear to the field direction. This assumption has proved a very useful one, but strictly speaking there is no general requirement of the collinearity between the field and the induced magnetic moment of atoms. The most important exception from this case represents magnetically anisotropic materials, where a non-collinear magnetic density distribution takes place in the presence of magnetic field. The main cause of the non-collinearity is the spin-orbit interaction by which the atoms spin directions are coupled to the orientation of its ligand environment. In case when the orbital moment is not fully quenched, the induced moments can in general be not parallel to the field.
It has been demonstrated recently that this "non-collinear" components of the induced magnetization can be determined using so-called "atomic site susceptibility parameters" method [1]. In the presentation recent results obtained using this approach will be given in comparison with some results of conventional spin density studies.

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MS24 O3

Observation of charge-density waves in $BaRuO_3$ using x-ray scattering Chao-hung Du,[a] K. J. Tseng,[a] Y. Y. Lo,[a] Mau-Tsu Tang [b], [a] *Department of Physics, Tamkang University, Tamsui 251, Taiwan.* [b]*National Synchrotron Radiation Research Center, Hsinchu 300, Taiwan.* E-mail: chd@mail.tku.edu.tw

Keywords: CDWs, Ferromagnetism, X-ray scattering

Studies of perovskites have stimulated research into a wide variety of unusual transition metal oxides, since the discovery of high T_C superconductors and CMR materials. It has been demonstrated that the interplay between the different degrees of freedom in perovskites can result in a very reach phase diagram, including the unusual conductivity and magnetism, charge/spin stripes, or even the phase separation phenomenon. The recently discovered layered ruthenate compounds have also been the subject of considerable study, especially for the discovery of superconductivity in Sr_2RuO_4. However, the mechanism the superconductivity in strontium ruthenates is still not clear, for example, the correlation between the dimensionality and the local moment [2, 3]. $BaRuO_3$ is chemically related to $SrRuO_3$, but displays different crystallographic forms. Therefore, it can be the model for understanding these issues. $BaRuO_3$ has been reported to show the unusual electrical and magnetic properties, and the pseudogap and charge-density waves (CDWs) were suggested to be the causes. The pseudogap has been observed using optical spectra [1], but the existence of CDWs was questioned because of lack of the experimental evidence. Using the x-ray *in-vacuum* camera on a high quality single crystal $BaRuO_3$, we located some weak spots at T= 30 K along the c^*-axis which doubles the c^*-axis of the unit cell. Further study using x-ray scattering, by measuring the peak profiles as a function of temperature, we observed that the CDW satellite reflections display a step-like transition at T≈ 80 and 50 K where the former is correspond to the formation of CDW, and the later could be caused by the lattice distortion which is related to a weak ferromagnetic transition as confirmed from susceptibility measurement.

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