European Science Foundation

Interdisciplinary Approaches to Functional Electronic and Biological Materials (INTELBIOMAT)

Exchange Visit Grant 4211

Scientific Report

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Title of the project: **NMR Study of the magnetic and electronic properties of layered cobaltates**
Host institute: **Laboratoire de Physique des Solides, Université Paris Sud, Orsay**, **France**
Date of visits: **2/05/2013-30/05/2013** and **3/07/2013-26/07/2013**
Length of stay : **7 weeks**

1. Purpose of the visit;

The aim of this visit to Laboratoire de Physique des Solides was to perform a detailed study of magnetic phase of sodium cobaltates with a T_N=22 K by ^{59}Co NMR. In 2011 in Kazan we have installed and put in operation the optical furnace for the floating zone growth of single crystals, which has allowed us to grow single crystalline sodium cobaltates Na_xCoO_2. So the necessary single crystals of T_N=22 K phase of sodium cobaltates was synthesized in Kazan before visit to Orsay. The unique sweep field magnet with maximum field 14 T in Orsay allows to perform precision ^{59}Co NMR measurements in the temperature range 4.2-300 K and to clarify the charge and spin state of cobalt ions specific to this phase.

2. Description of the work carried out during the visit;

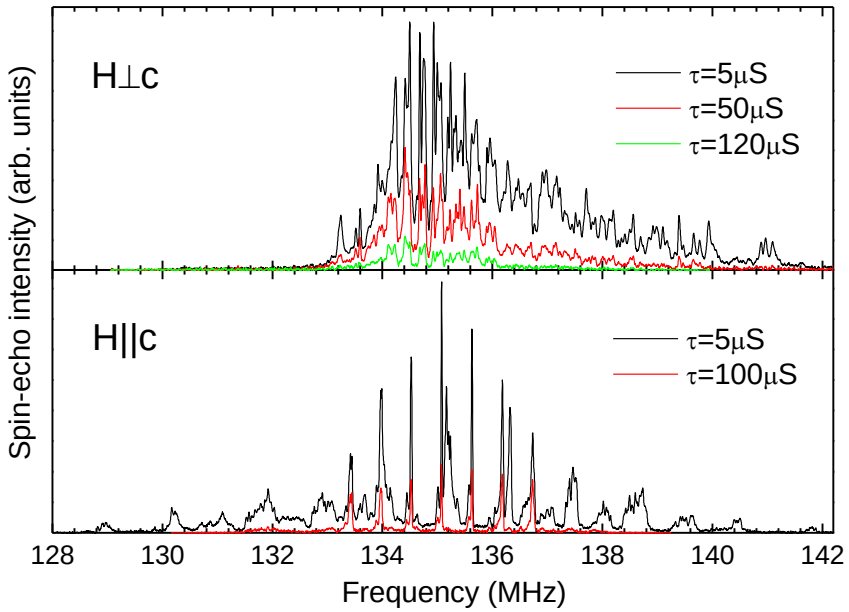
As it was proposed in the application we have splitted the stay in Orsay for two visits. The first visit (4 weeks) was in May 2013. During it using ^{59}Co NMR we found that the crystals which were grown in Kazan contain two phases of sodium cobaltates with slightly different sodium content. Using the electrochemistry cell we succeeded to homogenize the sodium content in the crystals and obtained a set of single crystals which contained only a single phase with T_N=22 K. After that the systematic ^{59}Co NMR measurements of these crystals were done. We found that the ^{59}Co NMR spectra of T_N=22 K phase is very broad so the sweeping field capability of the 14 T magnet in Orsay was a quite important to do our study.

After 1st visit in Orsay I returned back to Kazan and a new single crystal of sodium cobaltates were grown with some improvements the single crystal synthesis procedure. Also during my stay in Kazan the analysis of the obtained ^{59}Co NMR data were done.

During the 2nd stay in Orsay which was for 3 weeks in July 2013 we accomplished the analysis of the ^{59}Co NMR data and begun to prepare a paper with results of our Co NMR studies on the specific phase of sodium cobaltates with 22 K Néel temperature.

3. Description of the main results obtained;

Example of the ^{59}Co NMR spectra measured in the single crystal of sodium cobaltates with T_N=22 K at different experimental conditions and T=80 K is presented in next figure:



We succeed to resolve the 6 components in these spectra which correspond to the six unequivalent cobalt sites in the unit cell of this specific phase of sodium cobaltates with 22 K Néel temperature. These 6 components of the spectra differ by the quadrupolar splitting and basing on nuclear relaxation measurements can be grouped in 3 groups: slow relaxing Co1, intermediate Co2 (contains 3 components) and fast relaxing Co3 (2 components). The slow relaxing Co1 component of the spectra forms only about 23-25% of the total intensity of the spectra and corresponds to the non-magnetic Co^{3+} charge state. This experimental result precludes localized moments pictures for the magnetic properties of studied phase. In the $Na_{2/3}Co_2$ phase which we studied before charge disproportionation in the cobalt planes leads to a separation into slow relaxing and fast relaxing cobalts only. Therefore the charge disproportionation in the phase of sodium cobaltates with T_N=22 K is more complicated than in 2/3 phase.

Unexpectedly we found that Co2 and Co3 components of ^{59}Co NMR spectra have some substructure which shows that for this peculiar phase the 3 dimensional order is not perfect.

4. Future collaboration with host institution (if applicable);

We are pleased with the results gained from this exchange visit which permits us not only to finalize our work on the 22K phase, but also permits to drive the collaboration between Orsay and Kazan towards single crystal materials. We have in plans to perform systematic transport properties measurements of the sodium cobaltates single crystals with different sodium content in collaboration with F. Rullier-Albenque (Service de Physique de l'Etat Condens´e (CNRS URA 2464), CEA Saclay, France). Also the NMR study of other phases of sodium cobaltates in Orsay and Kazan will be continued.

5. Projected publications / articles resulting or to result from the grant;

The paper concerning our Co NMR studies on the specific phase of sodium cobaltates with 22 K Néel temperature was started during my visits and is currently in progress.