実験報告書様式（一般利用課題・成果公開利用）

MLF Experimental Report	提出日 Date of Report **July 9, 2013**
課題番号 Project No. 2013A0050 実験課題名 Title of experiment **Mechanism of the successive transitions of Ba ($Fe_{1-x}Co_x)_2As_2$** 実験責任者名 Name of principal investigator **Masatoshi Sato** 所属 Affiliation C o m p reh en sive R esearch O rgan izatio n F o r S cien ce an d S o ciety	装置責任者 Name of responsible person **Takashi Kamiyama** 装置名 Name of Instrument/ (BL No.) **BL-08** 実施日 Date of Experiment **May 9-14, 2013**

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）

Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

Samples:

In order to avoid effects of external stresses, we used samples consisting of assemblies of mm-size crystallites of $Ba(Fe_{1-x}Co_x)_2As_2$ with x = 0.0, 0.01 and 0.02, because the system was known to exhibit significant responses to external stresses. In our measurement, they were free, at least, from stresses originating from (1) surface effects, which may exist in finely pulverized samples, and from (2) effects of grease or other glues used to fix a single crystal sample to a holder. We also considered effects of impurities doped to the system, and therefore used samples both with and without Co impurities. The volume of each sample was (2-3) cm^3.

2. 実験方法及び結果 （実験がうまくいかなかった場合、その理由を記述してください。）

Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

Experimental method:

For each crystallite assemblies, data were taken at about 25 temperature points in the T region between 80 K and 300 K, where temperature was stabilized with an accuracy of about ±0.25 K. The measuring time was about 1 h at each T point. Then, observed intensities of the Bragg reflections were plotted against the d-spacing between 0.5-3.0 A, where we could take rather good data even though the very high resolution of $\Delta d/d$ (of the order significantly less than 10^{-3}) was required. For the samples with x=0.0 and 0.02, we could take a series of data in due course. For x = 0.01, measurements were carried out only for a half of planned T-points because of the stop of the beam supply during the allocated beam time.

Results:

The direct purpose of the measurements is to understand the T-x phase diagram of Ba $(Fe_{1-x}Co_x)_2As_2$, which contains three characteristic temperatures, the antiferromagnetic (AF) transition temperature T_N, so-called "tetragonal-orthorhombic transition point" T_S, and one more temperature T^* characterizing the break down of

2．実験方法及び結果（つづき） Experimental method and results (continued)

the C_4 symmetry even in the nominally “tetragonal” phase above T_S. (Note that $T_N \leq T_S < T^*$). The phase diagram attracts much attention, because to understand it seems to be the best way to find how the spin and orbital degrees of freedom determine this phase diagram, and to get useful clues to identify the superconducting mechanism.

Here, the significant softening of the elastic constant C_{66} found at T_S, and the strange breaking down of the C_4 symmetry in the region of $T_S \leq T < T^*$ have to be pointed out, because they indicate finite couplings between the lattice system and the two degrees of freedom mentioned above, suggesting that these couplings are also important ingredients for the determination of the phase diagram. (By the way, very sensitive nature of various physical properties of Fe-based superconductors to external stresses is possibly due to this lattice softening, which is the reason why we used the samples consisting of assembly of mm-size crystallites.)

Theoretically, two candidates mechanisms of the superconductivity based on spin and orbital fluctuations, have been proposed. Under this condition, we have studied how the lattice system behaves as T increases from the low T region through the three temperatures, in particular around T^*, and what we can report on the result of the experiment, at this moment, is as follows. Although we do not want to describe the details of the observed data here, strong indications that the behavior of the lattice system observed in the region above T_S does not seem to be intrinsic, and that the intrinsic tetragonal-orthorhombic structural transition takes place at T_S. Our data show, however, that the orbital degrees of freedom are involved in the determination of the phase diagram.