DUBBLE – EXPERIMENT REPORT

We kindly request you to answer the questions (max 2 pages) and return the form to NWO **within 2 months of the completion of the experiment** to **dubble@nwo.nl**

Beam time number: **26-01-1105**		**File number:** **195.068.1001**
Beamline: **BM01A**	**Date(s) of experiment:** **2-4 March 2017**	**Date of report:** **7 March 2017**
Shifts: **3**	**Local contact(s):** **Dmitry CHERNYSHOV**	

1. **Who took part in the experiments?** (Please indicate names and affiliations)
   Niels van Dijk - TU Delft
   Maurits Boeije – TU Delft
   Xinmin You – TU Delft

2. **Were you able to execute the planned experiments?**
   YES

3. **Did you encounter experimental problems?**
   NO

4. **Was the local support adequate?**
   YES

5. **Are the obtained results at this stage in line with the expected results as mentioned on the project proposal?**
   YES

6. **Are you planning follow-up experiments at DUBBLE for this project?**
   NO

7. **Are you planning experiments at other synchrotrons in the near future?**
   NO

8. **Do you expect any scientific output from this experimental session (publication, patent, ..)**
   YES. The results are planned to be published in a scientific publication and will be part of a PhD thesis. A publication is expected to be submitted within a year.

9. **Additional remarks**
   None

Charge density redistribution in magnetocaloric La(Fe,Co,Si)13 measured by powder diffraction

The $La(Fe,Si)_{13}$ class of materials exhibit a giant magnetocaloric effect (GMCE) and is attractive as a highly efficient and environmentally-benign technology for room-temperature magnetic refrigeration [1]. When heating these materials above the ferromagnetic transition temperature, the cubic structure undergoes a volume change. The origin of the volume change is attributed to a change in the size of the magnetic moments across the transition [2]. The same mechanism was found in Fe_2P-based materials [3], which is facilitated by the presence of two magnetic sublattices. As shown in Fig. 1, for Fe_2P based compounds the experimentally observed charge redistribution across the ferromagnetic transition (obtained by powder XRD) confirmed the density functional theory (DFT) calculations. Proving the similar nature of the transition in the $La(Fe,Si)_{13}$ system will complement our insight both material families and help in the development of these materials.

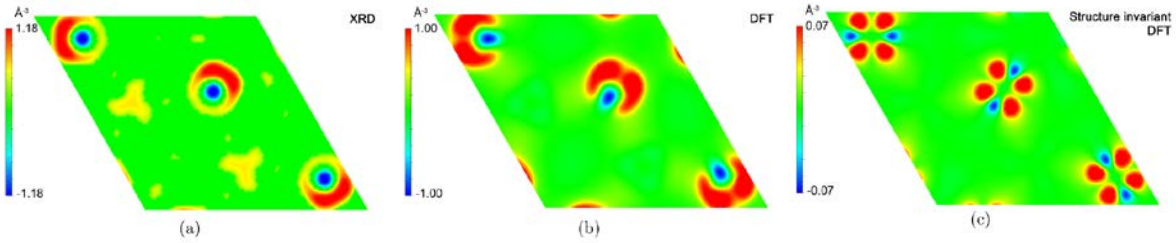

Fig. 1: *Difference between the electron densities above and below the Curie temperature in the Fe_2P system from (a) XRD experiments, (b) DFT calculations and structure-invariant DFT calculations* [3].

We have performed X-ray powder diffraction measurements at beamline BM01A with a photon energy of 17.9 keV on $La(Fe,Co,Si)_{13}$ samples as a function of temperature from 150 to 500 K, for both heating and cooling. The preliminary results show (1) a large discontinuous change in lattice parameters for the sample with a strongly first-order transition, (2) a moderate change in the sample with a weakly first-order transition and (3) a small continuous change in the sample with a second-order transition. The data will be used to perform a Fourier synthesis to generate electron density plots similar to the ones presented in Fig. 1 for Fe_2P-based alloys.

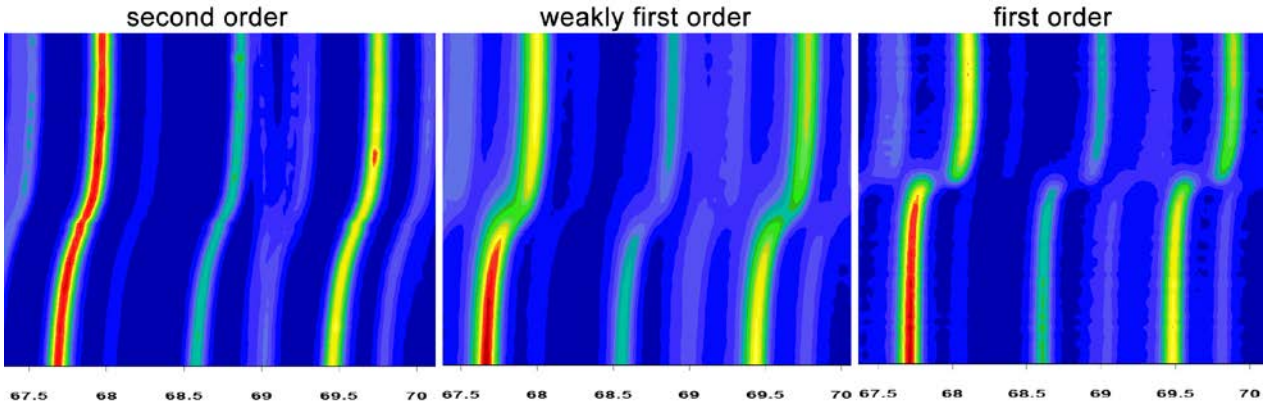

Fig. 2: Temperature evolution of the scattered intensity as a function of the diffraction angle (2θ) for $La(Fe,Co,Si)_{13}$ samples with a (*i*) second-order, (*ii*) weakly first-order and (*iii*) a first-order ferromagnetic-to-paramagnetic transition.

References

[1] A. Fujita et al., Phys. Rev. B 67 (2003) 104416.
[2] M. Gruner et al., Phys. Rev. Lett. 114 (2015) 057202.
[3] M.F.J. Boeije et al., Chem. Mater. 28 (2016) 4901.