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: **26-01-1042**		**File number:** **195.068.861**
Beamline: **BM01A**	**Date(s) of experiment:** **9-14 December 2015**	**Date of report:** **18 December 2015**
Shifts: **14**	**Local contact(s):** **Philip PATTISON & Dmitry CHERNYSHOV**	

1. **Who took part in the experiments?** (Please indicate names and affiliations)
   Niels van Dijk - TU Delft
   Maurits Boeije – TU Delft
   Michael Maschek – 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?**
   YES, depending on the detailed outcome.

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

Electron density redistribution in magnetocaloric $(Fe,Mn)_2(Si,P,B)$ measured by powder diffraction

The giant magnetocaloric effect (GMCE), associated with a first-order magnetic transition (FOMT), makes near room-temperature magnetic refrigeration attractive as a highly efficient and environmentally-benign technology [1,2]. We discovered the GMCE in the $(Mn,Fe)_2(P,Si)$ compounds. In this system the magnetic transition temperature can be tuned over a wide range of temperatures by varying the Mn/Fe and P/Si ratios [3]. Recent first-principle electronic-structure calculations on $MnFeP_{0.5}Si_{0.5}$ [3] indicate that at the first-order ferromagnetic phase transition a strong electronic reconstruction takes place (see Fig. 1).

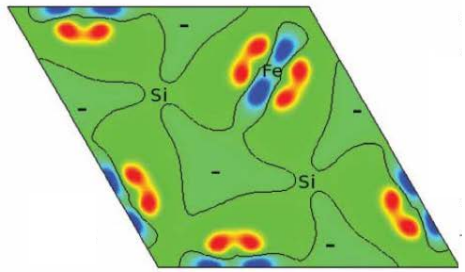

Fig. 1: *Difference between the electron densities calculated for situations above and below the Curie temperature in the iron-silicon/phosphorous plane* [3].

We have performed X-ray powder diffraction measurements at beamline BM01A as function of temperature (from 100 to 400 K) and applied magnetic field (up to 2 T). 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 Fig. 1.

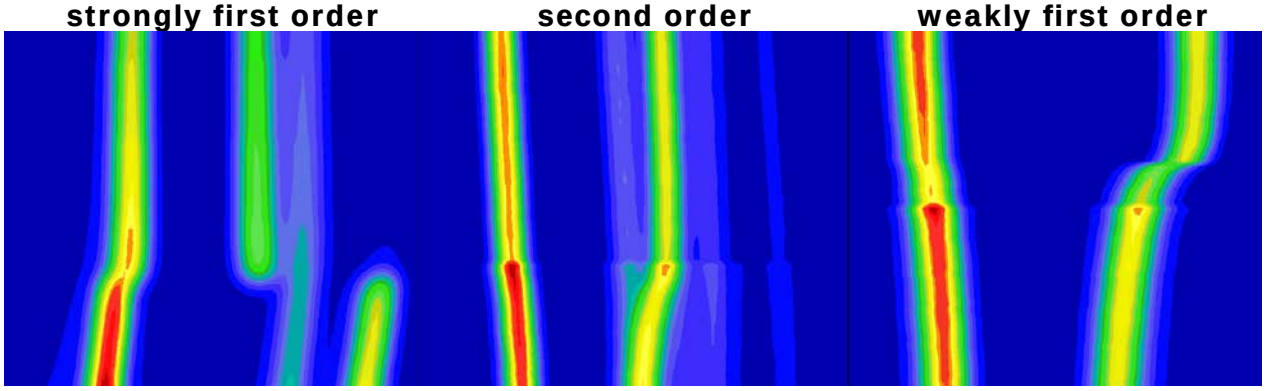

Fig. 2: Temperature evolution of the scattered intensity as a function of the diffraction angle ($2\theta \approx 20^{o}$) for the three different systems.

References

[1] O. Tegus , E. Brück , K. H. J. Buschow , F. R. de Boer, *Nature 415 (2002) 150 .*
[2] E. Brück, *Handbook of Magnetic Materials vol. 17, Elsevier (2008) 235*.
[3] N.H. Dung, Z.Q. Ou, L. Caron, L. Zhang, D.T. Cam Thanh, G.A. de Wijs, R.A. de Groot, K.H.J. Buschow, E. Brück, *Adv. Energy Mater. 1 (2011) 1215*.