ESRF	**Experiment title:** Investigation of structural chirality in $Fe_{1-x}Co_xSi$ and $Mn_{1-y}Fe_ySi$ compounds with Dzyaloshinskii-Moriya interaction	**Experiment number:** 01-02-853
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Report:

X-ray diffraction of single crystals under certain conditions also allows one to distinguish between left- and right-handed enantiomorphs. The corresponding technique based on the Flack parameter [1] has been applied to many compounds and is routinely used by crystallographers. The Flack parameter f can be expressed via half-difference of intensities of Friedel equivalents [1, 2]:

$$I(\mathbf{H}) - I(-\mathbf{H}) = (1 - 2f)(|F(\mathbf{H})|^2 - |F(-\mathbf{H})|^2). \quad (1)$$

Here I and F denote the intensity and the structural factor for the Bragg reflection $\mathbf{H}$, respectively. The Flack parameters may, therefore, be considered a measure of the ratio of domains of different handedness. A zero value of Flack parameter indicates an enantiopure sample with the correct absolute structure. For a Flack parameter equal to 1 the crystal structure has to be inverted. The ability of the x-ray diffraction experiment to distinguish between structures with opposite chirality originates from the resonance scattering contribution in the structural amplitudes. This contribution defines the wavelength-dependent inversion distinguishing power (IDP) [2], $|F(\mathbf{H})|^2 - |F(-\mathbf{H})|^2$. A simple estimation reveals that a wavelength $\lambda = 0.77$ Å provides sufficient IDP for many Bragg reflections.

The X-ray diffraction data were collected with synchrotron radiation with $\lambda = 0.77$ Å at the Swiss-Norwegian Beam Line BM01A using the KUMA6 diffractometer. Crystals with an average size about 50 microns were prepared from the same batches as was used before for the neutron scattering measurements. The absolute structure was found by refining the Flack parameter, together with the inspection of the inverted

structure. The structure of the etalon MnSi sample is identical to those found in the literature [3], with $u_{\mathrm{Mn}} = 0.135$ and $u_{\mathrm{Si}} = 0.845$.
The structure of the compound with $x = 0.10$ is identified as $P2_13$ with the structural parameters $u_{\mathrm{Fe/Co}} = 0.865$ and $u_{\mathrm{Si}} = 0.155$. For the compound with $x = 0.25$, $u_{\mathrm{Fe/Co}} = 0.138$, and $u_{\mathrm{Si}} = 0.846$. Low R factors ($x = 0.10$, $R_1 = 1.8\%$, $wR = 3.8\%$ and $x = 0.25$, $R_1 = 1.7\%$, $wR = 4.3\%$) together with a well-defined Flack parameter of the order of 0.00(6) confirm that the absolute structure has been determined correctly. With the absolute structure the crystallographic chirality of a helix propagating along a given direction can easily be determined.
We found that the congruent crystal handedness of MnSi and $Fe_{1-x}Co_xSi$ produces the opposite magnetic chirality and vice versa. We have proved that the structurally left samples of $Fe_{1-x}Co_xSi$ (with $u_{\mathrm{Me}} = 0.138$, $u_{\mathrm{Si}} = 0.846$) drive right-handed clockwise spin helices and right samples (with $u_{\mathrm{Me}} = 0.865$, $u_{\mathrm{Si}} = 0.155$) make the acticlockwise helices. This situtation is opposite to the case of MnSi where a left-handed crystal generates left-handed anticlockwise magnetic spirals. These two types of the compounds are clear to posses different signs of the Dzyaloshinskii-Moria interaction constituting their spiral structure [4]: negative sign (−) for MnSi type and positive sign (+) for $Fe_{1-x}Co_xSi$ type. We guess it would be really interesting to study whether and how the different Dzyaloshinskii sign affects the magnetic properties of the compounds with the same Co concentration.
Analysing all these facts we can make a conclusion that the chirality of the $Fe_{1-x}Co_xSi$ solid solutions does not depend on the Co concentration, but it is determined by the the seed's chirality which can be called as the inherited parameter. However, certain mistakes incipient during the growth process may flop the chirality of the future crystal.

References

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[4] Båk, P. and Jensen, M. H. (1980) *Journal of Physics C: Solid State Physics* **13(31)**, L881.