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The X-ray and polarized neutron diffraction are used to determine the crystal handedness and magnetic chirality of the series of high-purity MnSi single crystals and mixed compounds crystals of $Mn_{1-x}Fe_xSi$ and $Fe_{1-x}Co_xSi$ grown by Czochralski methods [1,2]. To test the possibility to control the crystal handedness of the single crystals we have performed the following experiments with the crystal growth using Czochralski technique. (i) Using as a seed the right-handed crystal $Fe_{1-x}Co_xSi$ with $x = 0.10$ we have grown one series of $Fe_{1-x}Co_xSi$ samples with $x = 0.10, 0.15, 0.20, 0.25, 0.30, 0.50$. (ii) Using as a seed the left-handed crystal with $x = 0.50$ we have grown another series of $Fe_{1-x}Co_xSi$ samples again of different concentrations. The result of these experiments aimed to demonstrate whether handedness of these crystals depends on the concentration of Co, or, it is solely determined by the seed used for this synthesis. The third option could be if the handedness would not depend on a seed and/or concentration x .

In 90% cases the grown sample has been found to be enantiopure and to inherit the crystallographic chirality of its seed crystal. In 10% cases undefined circumstances flip the chirality over for the next progeny or produce a racemic sample. We demonstrate that (i) left and right forms of all transition metal monosilicides can be grown by the Czochralski method, (ii) the magnetic chirality of all $Mn_{1-x}Fe_xSi$ crystals follows its crystallographic counterpart [1], (iii) the opposite coupling between the crystal handedness and the spin chirality has been found for $Fe_{1-x}Co_xSi$ compounds [2].

Knowing the rigid coupling between the structural handedness and magnetic chirality we used the polarised neutron diffraction to indirectly determine the average handedness of six different polycrystalline samples of MnSi with large number of crystallites (100 crystals per cm^3). The average chirality of these polycrystals deviates unexpectedly high from zero. This net chirality is maybe related to the yet poor statistics in the numbers of the left or right crystallites inside the polycrystals.

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Non-centrosymmetric molecules - centrosymmetric structure?

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It is recognized that macroscopically centrosymmetric crystal structures can still give rise to NLO phenomena, due to growth-induced polarization [1]. We can take this one step further, and look at molecules which conformationally, due to their synthesis, inherently are a mixture of centrosymmetric and non-centrosymmetric forms. If the conformational differences are very small, one would in such a case normally come to expect a completely disordered, centrosymmetric crystal structure.

The compound being discussed in this contribution, a double

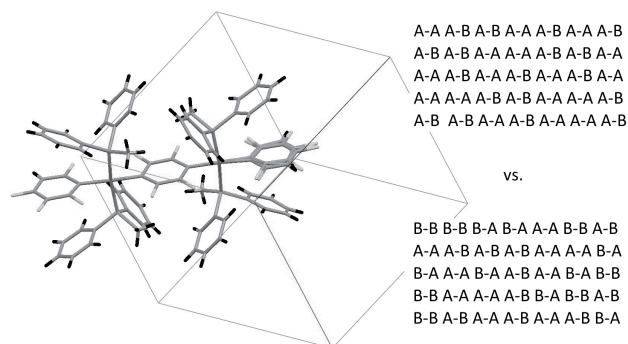
square planar Ni-phenylene complex [2] with 2,3,4,6-F-substituted phenyl rings that are unable to rotate once they bind to the complex, is ideally suited for this kind of study.

At first sight the compound indeed crystallizes in the space group P-1. We will explore the possibilities for experimentally exposing by x-ray crystallography the presence or absence of additional ordering within the crystal by way of growth-induced polarization, as well as the crystallization possibilities that such a substance really has.

These crystallization options for an A-A/A-B type compound consist of either a homogeneous, centrosymmetric, completely disordered structure (see figure, bottom); a racemic twin (i.e. polarization) with a (slight) preference for a particular orientation of one of the two rings; or else what is in fact a completely ordered structure on the molecular level, only allowing for disorder due to the statistical distribution of the second fluorinated ring. This would lead to the existence of large, completely ordered racemic twin domains within the crystal (see figure, top).

The presence or absence of this latter phenomenon would provide details on the process of crystal growth in this particular case.

We will here present the results, which indicate that centrosymmetry is not always what it appears to be at first sight. We have been able to deduce perfect ordering in the growth direction by re-examining different fragments of the same crystal, thus demonstrating that the resulting twin components are different in different regions of the same crystal, and that one ring is in fact completely ordered in domains that are macroscopic.



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Influencing absolute structure determination

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It is well established that the different enantiomers of a chiral material can have significantly different physiological properties. There are many well known, often quoted examples including the terpenes limonene & carvone [1], and the pharmaceuticals ibuprofen, naproxen and thalidomide [2]. As a consequence of this, drug manufacturers and drug authorisation authorities are increasingly concerned about the absolute configuration of active pharmaceutical ingredients. There are a number of "sporting" techniques, but one of the most relied upon is X-ray structure analysis [3], which in appropriate cases can give very reliable results.

The first absolute structure determination, of sodium rubidium