Structure / properties relationships in doped MgB_2 single crystals

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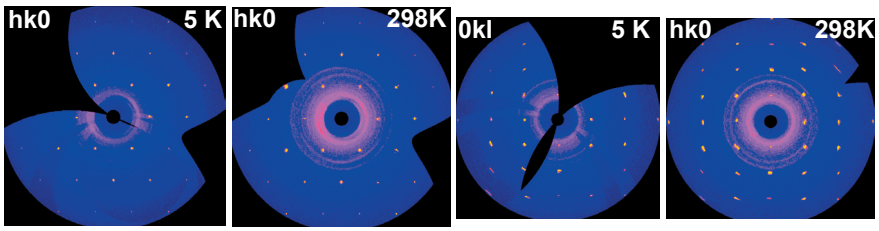
Pure MgB_2 single crystals at 5K



Reconstructed images of zero reciprocal space layer (l = 0); Imaging Plate measurements of pure MgB_2 single crystals at 298 K and 5 K with STOE IPDS; Mo $K_{\alpha 1}$; 300 s exposure time; $\Delta\varphi$ = 1°; dd = 150 mm.

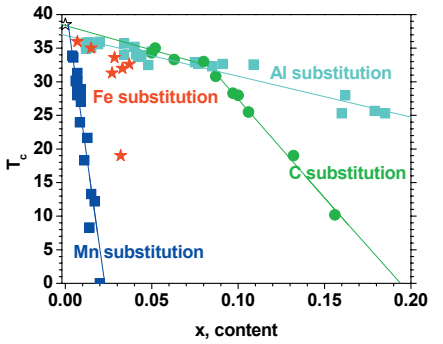
Investigation of possible structural changes in MgB_2 single crystals, which are correlated with superconducting properties (T_c= 39 K), measured with STOE IPDS Imaging Plate at 5 K and 298 K.

- **No phase transformation down to 5 K**
- **No additional reflections or splitting**

298 K: 189 (18) reflections; R_1 = 0.033, wR = 0.077

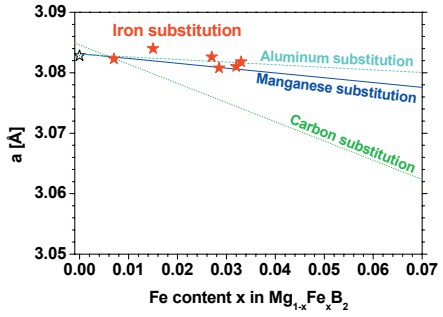
5 K: 192 (20) reflections; R_1 = 0.064, wR = 0.142
(Bad residual due to He inside Si-sample-tube)

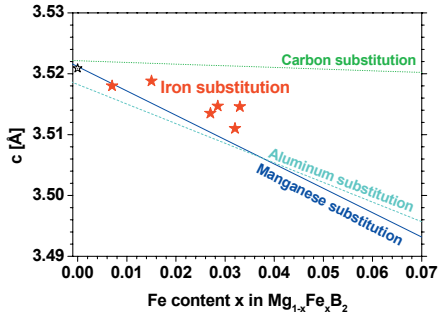
Doped MgB_2



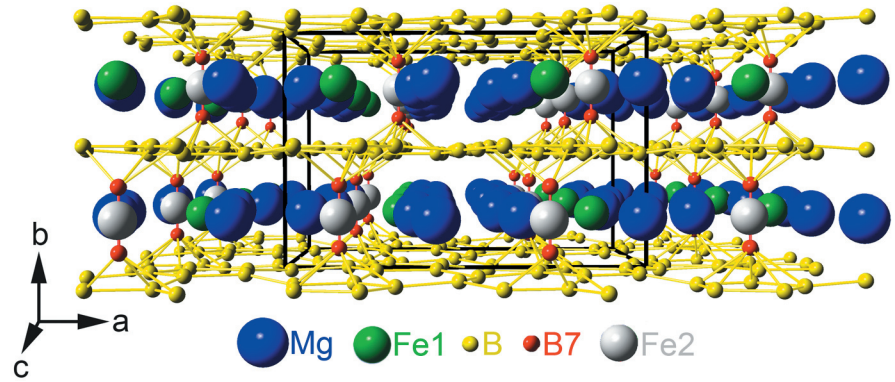
T_c dependence on Fe content, determined by EDX.

- **T_c(x) behaviour of Fe doped MgB_2 crystals** differs from that of Mn doped MgB_2 single crystals [1], possibly due to "second phase" effect.
- **Lattice constants behaves as for Al or Mn doped crystals --> Fe on Mg position**

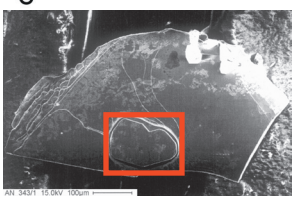




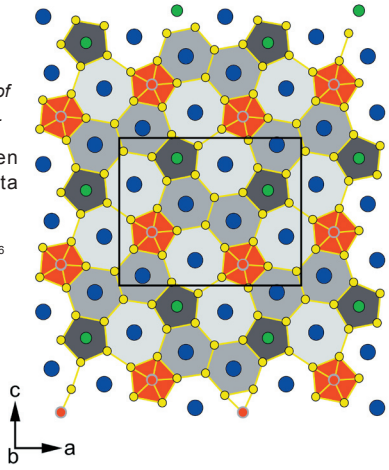
New compound in the Mg-Fe-B system



Boron layers alternate with Mg-Fe layers; Fe1 (top: drawn in green) position is fully occupied, Fe2: occupation ≈ 10%; (top: drawn in grey), either Fe2 or B7 is occupied (B7: occupation ≈ 90%); B7 (top: drawn in red) is connected to the five-membered boron rings (below: drawn in red); B7-B7 = 1.674(3) Å.



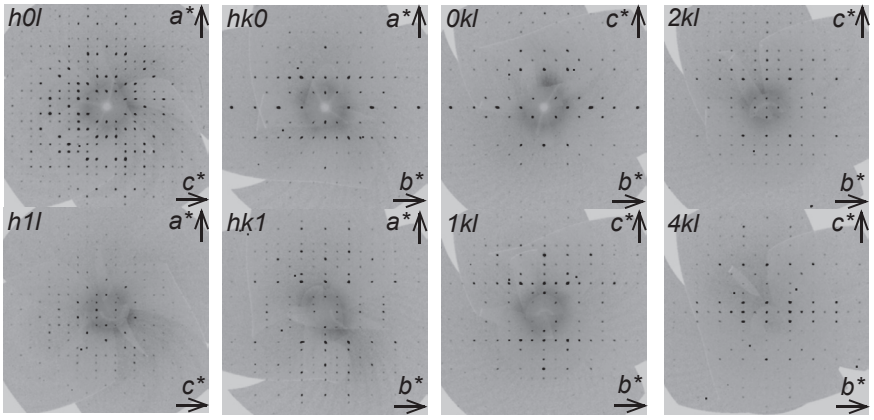
SEM image of a $Mg_{1-x}Fe_xB_2$ crystal with the inclusion (red area) of the new Mg-Fe-B phase (composition from EDX: ≈ $Mg_{0.75}Fe_{0.25}B$).



The structure of a new Mg-Fe-B compound has been solved tentatively from single crystal X-ray data (SMART CCD, Mo$K_{\alpha 1}$):

- Boron network (5-,6-,7-membered rings) similar to Y_2ReB_6 a = 11.28 Å, b = 8.94 Å, c = 3.39 Å, Pbam (No.55) [2].
- $Mg_4Fe_{1.1}B_{13.9}$, doubling of b (corresponds to c in Y_2ReB_6)! a = 10.95 Å, b = 7.07 Å, c = 8.72 Å, Pnma (No. 62).
- 1410 reflections,114 parameters, R_1= 0.021, wR = 0.049 R_{int} = 0.030 S = 1.052, $\Delta\rho_{max}$= 0.61 and $\Delta\rho_{min}$ = -0.33 eÅ^{-3}

The apparent mutually exclusive Fe2, B7 occupation result requires further study (twinning ?...).



Reconstructed images of reciprocal space layers; CCD measurements of the new Mg-Fe-B compound single crystals with SMART CCD; Mo $K_{\alpha 1}$; 60 s exposure time; $\Delta\varphi$ = 0.3°; dd = 30 mm.

References

[1] K. Rogacki et al., in preparation.
[2] Y. Kuz`ma et al., Z. Krist. NCS, 218, 159 (2003).

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