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Revealing the faulted structure of α -FeB and its implications

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Abstract

Iron borides are a family of materials that has attracted considerable attention due to its properties relevant to the fields of powder metallurgy, magnetism, catalysis and metal-air batteries.[1] The compositions cover a wide range from Fe₉B to FeB₄₉, out of which Fe₂B and β -FeB outstand as well-described thermodynamic phases.[2] The low temperature modification of the former, so-called α -FeB, can be synthesized as nanostructures of different sizes and shapes, which has opened the door to the tailoring of specific properties.[2] For instance, nanosized α -FeB displays a very open magnetic hysteresis, in contrast to the soft ferromagnetism of β -FeB, relevant for applications in data storage.[3] A big problem for the fundamental research of α -FeB though, is the fact that its structure is not well understood, which obstructs results interpretation. The discord lies in the fact that the powder diffractogram of α -FeB resembles that of β -FeB, with the exception that some Bragg reflections are missing (Figure 1). Several models have been suggested to explain these features: (i) a point defect modification of β -FeB where the B and Fe atoms are exchanged, (ii) the crystallization in the CrB structure type of space group Cmc₂m and (iii) a random stacking between CrB and β -FeB structure types.[3] However, none of the models has been critically examined nor proved to reproduce an experimental diffraction dataset.

In the present work we have synthesized and deeply characterized the structure of α -FeB. All structure propositions are exhaustively analyzed. Electron microscopy images, shown in the inset of Figure 1, suggests the presence of stacking faults as the most plausible model. Indeed, while no accurate agreement was obtained for models (i) and (ii), model (iii) explains the experimental diffractogram. The stacking faults model was built on the basis of 4-layer types of β -FeB, each corresponding to different origin choices, such that, depending on the stacking sequence, β -FeB or CrB-type clusters are formed (Figure 1 inset). The average interference wavefunction from each layer is computed by exploiting the recursive nature of the patterns found in randomized stacking sequence. The powder pattern is modelled as a function of the faults probability (p), as shown in Figure 2. It can be seen that for an intermediate faulted system, the simulated pattern reproduces the corresponding absences in the experimental diffractogram, thus putting an end to the long-standing structural controversy. Examples of the implications of the faulted structure for the chemical use of FeB will be discussed.

References

[1] Wei, Y., et al. J. Mater. Res. (2017), 32, 883. [2] Rades, S., et al. ChemPhysChem. (2011), 12, 1756. [3] Rades, S., et al. Chem. Mater. (2014), 26, 1549.

Figure 1.

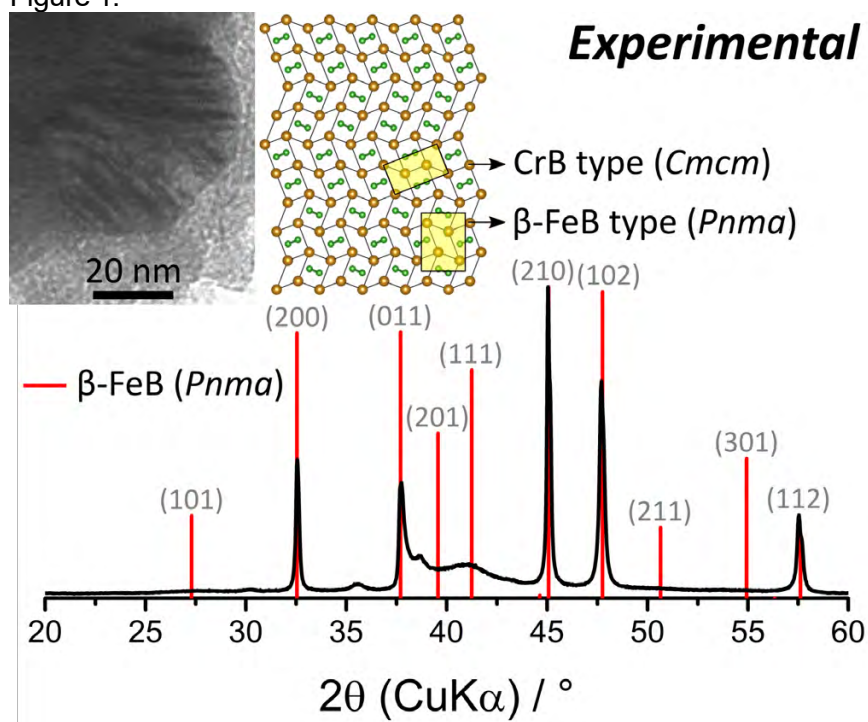


Figure 2.

