Influence of polytype formation and Al and Si ordering on the crystal structure in β-$Al_{4.5}FeSi$

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The β-$Al_{4.5}FeSi$ phase accompanied by δ-Al_3Si_2Fe [1] occurs as plate-shaped intermetallic particles in secondary, i. e. Fe-containing hypoeutectic Al-Si alloys that have formed during solidification or during heat treatment. A clear identification of the β phase within the microstructures is required for a thorough and correct investigation of the actual samples and, thus, further interpretation of the microstructure with respect to the processing and properties. However, at the different scales unsolved issues of the atomic crystal and defect structure obstructs appropriate interpretation of certain structural features of the β phase. This has consequences for (1) the phase identification, interpretation of (2) the morphology of the particles, (3) line-like contrasts within the particles at the micro- and nano-scale and (4) additional reflections or streaking reflections as well as peak-splitting observed by diffraction.

The present study reconciles experimental results, own and from literature. New theoretical evidence from DFT calculations is provided in order to conclude on unsolved issues of the structure interpretation with consequences at all microstructural levels. The new DFT calculations on the ordering of Al and Si atoms following up the results from Fang et al. [2] reveal complex characteristics of the ordering of Al and Si atoms.

It is concluded that the β-$Al_{4.5}FeSi$ phase locally occurs in a variety of ordered structures based on stacking of the constituting layers and the ordering of Al and Si atoms. Energetical preference is shown and experimental evidence is given for the AB polytype with two types of ordering of Al and Si atoms in space groups $A2/a$ and $P2_1/b$ as well as for the ABCD polytype. Additionally, locally disordered regions are observed. The consequences of the presence of these structures on the interpretation of characteristic from (1)-(4), observed phenomena is discussed.

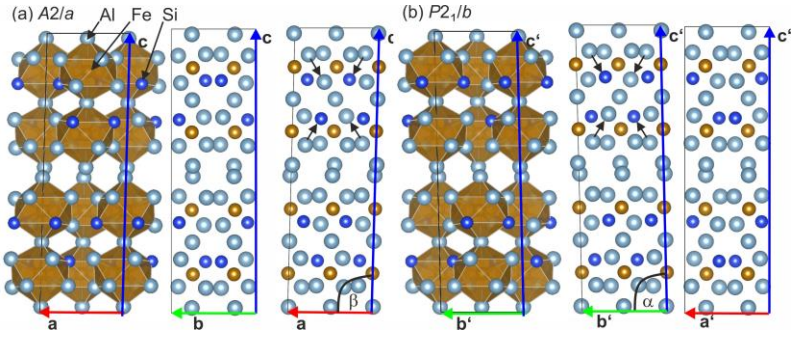

Figure 1: The two most energetically favored structures resulting from DFT calculations (a) in space group $A2/a$ and (b) in space group $P2_1/b$. The arrows point out where the ordering of Al and Si atoms enforces the monoclinic distortion. Note that the stacking sequence is AB in (a) and (b).

[1] Becker H, Bergh T, Vullum P. E, Li Y, Leineweber A. Journal of Alloys and Compounds, 780, 917-929, (2019).

[2] Fang C M, Que Z P, Fan Z. Crystal chemistry and electronic structure of the β-AlFeSi phase from first-principles, Journal of Solid State Chemistry, 299, 122-199, (2021)

The authors acknowledge support by DFG within the Collaborative Research Centre 920 "Multi-Functional Filters for Metal Melt Filtration—A Contribution towards Zero Defect Materials" (Project-ID 169148856) in sub-project A07.