EBSD studies on iron-rich U_xFe_yB_z compounds

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Borides play an increasingly important role in the present day engineering due to their high melting temperatures and chemical and thermal stability. A special case of interest is the ternary intermetallic borides of $A_xM_yB_z$ type (A=Actinide or Rare Earth, M=d-transition metal), with varying composition, as they have fascinating physical and chemical properties [1]. Their interesting physical properties extend from permanent magnetism with unusually large magnetic coercive fields, like in SmCo₄B [2] to unconventional magnetic ordering or superconductivity, as seen in UNi₄B [3].

Recent results on the U-Fe-B isothermal section at 950°C showed the existence of three new compounds, UFe₄B, U₂Fe₂₁B₆ [4] and UFe₂B₆ [5], in addition to the previously reported UFeB₄ and UFe₃B₂ [6,7]. The detailed knowledge of the B-Fe-U ternary phase diagram is essential for a comprehensive understanding of its ternary borides solidification behavior. A previous study on the B-rich region of the B-Fe-U phase diagram evidenced 18 boundary lines and 6 invariant reactions [8], the results on the Fe-rich region [9] showing the existence of additional 19 boundary lines and 10 invariant reactions. However, UFe₄B and U₂Fe₂₁B₆ compounds were observed to exist only as minor phases, both in the as-cast and in the annealed samples. Single crystals of the UFe₄B and U₂Fe₂₁B₆ compounds have never been isolated and the fact that these compounds do not melt congruently and have reduced primary crystallization fields [9] has hindered the production of single-phase polycrystalline materials. As a result, single crystal X-ray diffraction or powder X-ray diffraction (PXRD) data suitable for crystal structure refinement has so far not been collected for these two compounds.

The present work aims to further investigate the crystal structure of the $U_2Fe_{21}B_6$ and UFe_4B ternary borides. PXRD, scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and, especially, electron backscattered diffraction (EBSD) have been used with that purpose. The results showed that $U_2Fe_{21}B_6$ adopts the cubic $Cr_{23}B_6$ -type structure (*Fm3m* space group), while the UFe_4B crystallizes with a structure similar to the hexagonal $Lu_5Ni_{19}B_6$ -type (*P6/mmm* space group) as presented in Figure 1.

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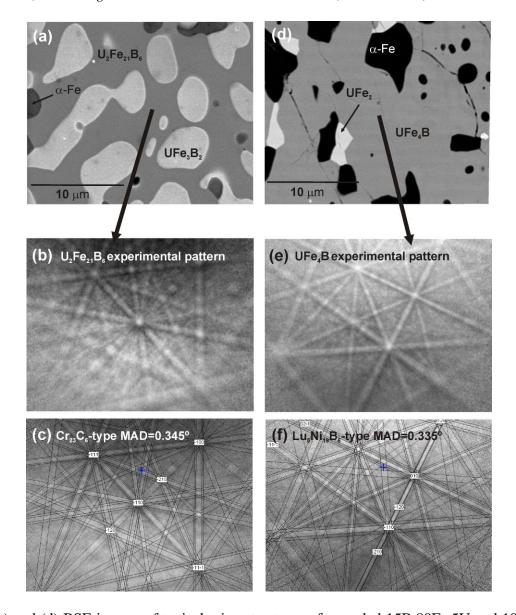


Figure 1 – (a) and (d) BSE images of typical microstructures of annealed 15B:80Fe:5U and 10B:80Fe:10U alloys, respectively, (b) representative experimental EBSD patterns annealed 15B:80Fe:5U sample in the $U_2Fe_{21}B_6$ phase and correspondent simulation for (c) $Cr_{23}B_6$ type structure, and (e) representative experimental EBSD patterns for annealed 10B:80Fe:10U sample in the UFe₄B phase and correspondent simulation for (f) $Lu_5Ni_{19}B_6$ type structure.