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Considerations on the U-Fe-B ternary system

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Uranium based intermetallic compounds frequently show unusual ground states and behaviours, such as unconventional superconductivity, coexistence of magnetic order and superconductivity, heavy fermion behaviour, etc. Ternary intermetallic borides of AM_xB_y type (A = actinide or rare earth; M = d-transition metal) have also attracted considerable interest due to their large diversity of physical characteristics, which extend from permanent magnetism with high coercive fields (like in $SmCo_4B$) to unconventional magnetic ordering (as seen in UNi_4B). However, the study of the U-Fe-B ternary phase diagram was far from being complete. Partial results on the isothermal section at 800°C for this system were first reported, with the identification of two compounds, $UFeB_4$ and UFe_3B_2 [1,2]. In this contribution we will present an overview of our recent work on the U-Fe-B ternary system, including the study of its isothermal section at 950°C, the liquidus projection and selected vertical section.

Over 70 alloys, with general $xU:yFe:zB$ compositions, were prepared by arc-melting the desired amounts of the elements, the melting process being repeated at least three times in order to ensure homogeneity. No losses higher than 1 wt.% were observed. The high cooling rate of the solidification process enabled to follow the solidification path of the alloys under non-equilibrium conditions. Subsequent heat treatments at 950 °C allowed inferring the transitions leading to equilibrium. The as-cast and annealed alloys were characterized by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), complemented with Energy Dispersive Spectroscopy (EDS), electron microprobe micro-analysis (EPMA), differential thermal analysis (DTA) and Electron Backscatter Diffraction (EBSD). Single crystal X-ray diffraction studies were also performed for some of the ternary compounds.

The U-Fe-B ternary system is considerably richer than what was reported before. A total of five ternary compounds were identified at 950°C: in addition to the previously reported $UFeB_4$ and UFe_3B_2 , three new compounds, UFe_4B , $U_2Fe_{21}B_6$ and UFe_2B_6 were found to be stable at this temperature. However, all these ternary compounds are formed by peritectic reactions, being difficult to obtain as single phase samples. Moreover, only for the $UFeB_4$, UFe_3B_2 and UFe_2B_6 compounds it was possible to get small single crystals suitable for X-ray diffraction studies. They have confirmed that $UFeB_4$ and UFe_3B_2 crystallize in the $YCrB_4$ and $CeCo_3B_2$ -type structures, respectively, and indicated that UFe_2B_6 is isostructural with the $CeCr_2B_6$ -type [3]. Moreover, in the case of the $UFeB_4$ compound it was found a cooperative (concomittant ?) growth of the $YCrB_4$ and $ThMoB_4$ type structures. For the other compounds, only PXRD measurements could be done, which indicate that UFe_4B crystallizes in a structure type related to the $CeCo_4B$ -type and that $U_2Fe_{21}B_6$ most probably crystallizes in the $Cr_{23}C_6$ -type. In order to get more information on the crystal structures of these last two compounds, EBSD studies were performed. They show that $U_2Fe_{21}B_6$ really crystallizes in the $Cr_{23}C_6$ -type structure and that the pattern of UFe_4B is better explained by the $Lu_5Ni_{19}B_6$ -type simulation.

A cascade of peritectic reactions was found to exist along the $U:(Fe,B)=1:5$ line [4]:

L + UB₄ UFeB₄
L + UFeB₄ UFe₃B₂
L + UFe₃B₂ UFe₂ + UFe₄B

The solidification paths show that the formation temperatures of the compounds decrease in the above order. Solidification ends with the ternary eutectic of UFe₂ + UFe₄B + β -Fe at 980 °C. The liquidus surface of the U-Fe-B ternary system is complex, with the presence of at least eighteen invariant points. The UFeB₄ and UFe₃B₂ have large primary crystallization surfaces, but for the other three compounds they are small and are far from their nominal composition. All this information represents fundamental knowledge for the synthesis of pure compounds, necessary for the physical properties characterization.

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