High-pressure studies of a ThMn$_{12}$-type actinide compound: UFe$_5$Al$_7$

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Abstract

The ternary inter-metallic compound, UFe$_5$Al$_7$, crystallize in a tetragonal ThMn$_{12}$ type structure. In the as-cast samples a residual phase of FeAl ($\sim$2% wt) was identified in the grain boundaries. The amount of the residual cubic phase of FeAl was determined by Rietveld analysis and reduced by the annealing process.

   UFe$_5$Al$_7$ maintains the tetragonal symmetry as a function of pressure, while FeAl keeps the cubic structure as was determined by the Rietveld analysis. The volume–pressure curve calculated from the x-ray analysis is $V/V_0 = 0.87$ for UFe$_5$Al$_7$ at 26.0 GPa.

1. Introduction

Many of the binary and ternary intermetallic compounds AB$_{12}$ and A(B$_x$C$_{1-x}$)$_{12}$ crystallize in the tetragonal ThMn$_{12}$-type structure [1]. In this structure the 2a sites are occupied by the A atoms while the three non-equivalent sites 8f, 8i, and 8j accommodate B and the C atoms according to special site preferences. The compounds of this group for which A is a rare earth or an actinide element (Re, An) and B and C are 3d transition elements are of special interest due to their potential use as permanent magnets.

   Binary ReFe$_{12}$ compounds do not exist and the above-mentioned magnetic compounds can be stabilized only as ternary compounds. Of these compounds the Re(Fe$_x$Al$_{1-x}$)$_{12}$ compounds exist for $4 \leqslant x \leqslant 7$ [2, 3]. In the present work the structural variation of the UFe$_5$Al$_7$ ternary intermetallic compound as a function of applied pressure was investigated.
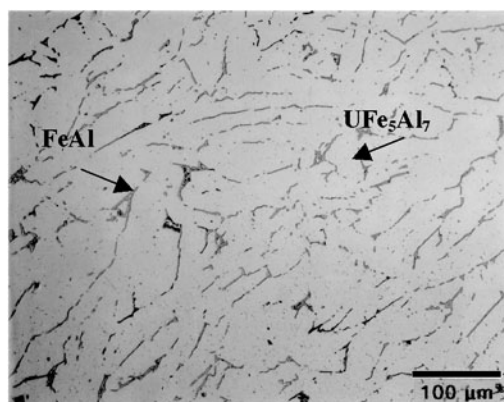
Figure 1. The morphology of this sample including the two different regions: UFe$_5$Al$_7$ and FeAl in the 800 °C heat-treated sample.

2. Experimental details

The sample, UFe$_5$Al$_7$, with nominal composition was prepared by arc-melting of stoichiometric amounts of the constituents under an argon atmosphere. The sample was annealed in an evacuated quartz tube and heat treated at 800 °C for 160 h. The microstructures were examined by SEM and the phases were analysed by EDS to determine their chemical compositions. Vickers micro-hardness tests were carried out.

X-ray powder diffraction measurements, angle and energy dispersive, were taken at ambient and high pressure (up to 26 GPa), using a Merrill–Bassett-type diamond anvil cell (DAC). The experiments were carried out in a 'Tel-Aviv'-type DAC with 500 μm culets. The pressure was calibrated with the ruby fluorescent technique [4]. The powder sample was held in Si oil as the pressure medium in a 250 μm diameter stainless steel gasket.

3. Results and discussion

Morphology of the structure

UFe$_5$Al$_7$ and Fe–Al ($\sim$2 wt%) were identified in the as-cast sample in the electron microscope micrograph. Large grains of UFe$_5$Al$_7$ were observed, while in the grain boundaries a FeAl phase [5] was identified; figure 1. The amount of FeAl phase decreased with the annealing process.

Micro-hardness tests

The hardnesses of the UFe$_5$Al$_7$ and the FeAl phases are 79.9(2.5) and 66.6(4.7) kg mm^{-2}, respectively, for the 800 °C heat-treated sample. This is higher by an order of magnitude compared with Al ($\sim$35–48 kg mm^{-2}) and U ($\sim$187–250 kg mm^{-2}) [6, 7].

X-ray

The powder diffraction spectra of the sample treated at 800 °C for seven days taken using Cu Kα radiation and a SiO monochromator are shown in figure 2.

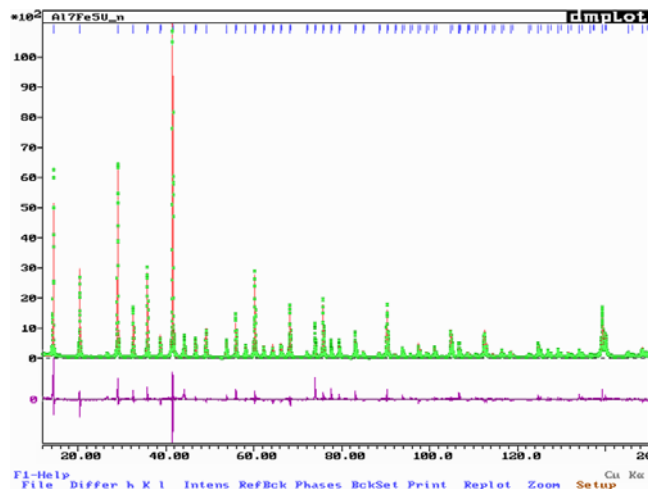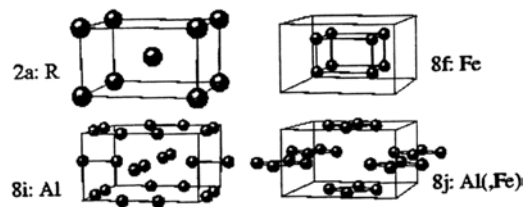**Figure 2.** The powder diffraction spectra of UFe$_5$Al$_7$ at ambient pressure.

Figure 3. The four partial structures of UFe$_5$Al$_7$ of the R(Fe, Al)$_{12}$ type.

Table 1. Structural parameters of UFe$_5$Al$_7$.

	UFe$_5$Al$_7$		
	0 GPa	11.5 GPa	20.6 GPa
a (Å)	8.696	8.459	8.201
c (Å)	5.020	4.841	4.721
c/a	0.577	0.572	0.575
V (Å^3)	379.61	346.40	317.52
X (8i)	0.342	0.342	0.342
X (8j)	0.285	0.284	0.283

ThMn$_{12}$-type structure of the R(Fe, Al)$_{12}$ (R = rare earth or actinides) intermetallics is described by the tetragonal space group $I4/mmm$. The unit cell contains two formula units and is composed of four partial structures formed by R in the 2a $(0, 0, 0)$, Fe in the 8f $(0.25, 0.25, 0.25)$, Al in the 8i $(x, 0, 0)$ and Al/Fe in the 8j $(x, .5, 0)$ sites (figure 3).

The x-ray diffraction measurements indicate a main phase of UFe$_5$Al$_7$ and a residual phase of FeAl [5] in agreement with the above references and the morphology. Rietveld [8] analysis with $R = 10\%$ indicates that the UFe$_5$Al$_7$ compound has a ThMn$_{12}$-type, $I4/mmm$ symmetry tetragonal structure with the lattice parameters $a = 8.6963(9)$ Å and $c = 5.0205(8)$ Å. This low-uranium-content compound exhibits a large interatomic U–U distance, well beyond the Hill limit.
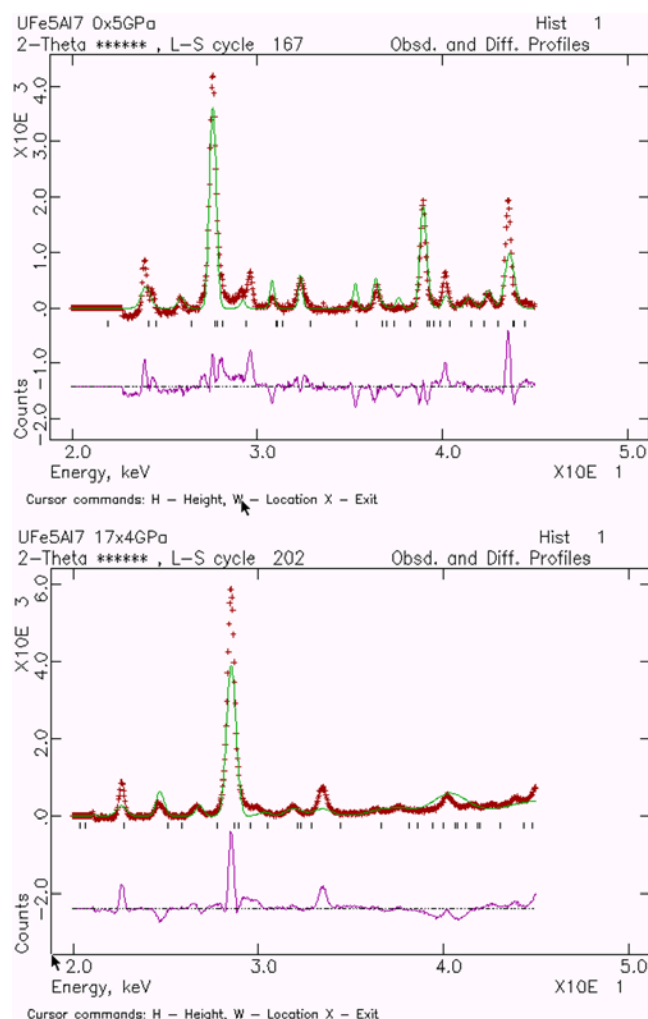
Figure 4. The powder diffraction spectra of UFe$_5$Al$_7$ at 0.5 and 17.5 GPa.

The amount of the residual phase of FeAl was determined by a Rietveld analysis as 2 wt%
±1 of the sample. The amount of the FeAl phase in the sample decreased upon annealing
as was indicated by x-ray diffraction and morphology. This is consistent with the previous
results. The lattice parameter of this phase is $a = 2.909$ Å, with $R = 11.7\%$.

X-rays under pressure

The UFe$_5$Al$_7$ maintains the tetragonal symmetry as a function of pressure, as was determined
by the Rietveld analysis; figure 4. The volume–pressure curve calculated from the x-ray
analysis is given in figure 5. $V/V_0 = 0.83$ at 26.0 GPa.

The unit cell and the atomic positional parameters are compiled in table 1. They are the
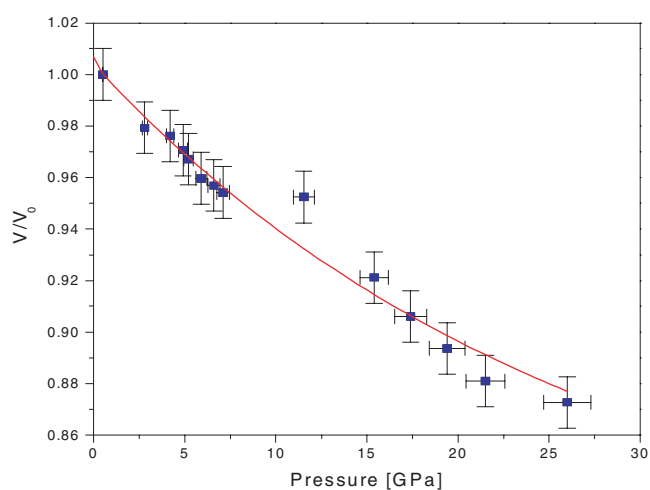results from the Rietveld analysis.

Figure 5. The volume–pressure curve for UFe$_5$Al$_7$.

References

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