

## UFe<sub>2</sub>Zn<sub>20</sub>: a new uranium intermetallic compound

A.P. Gonçalves<sup>a,\*</sup>, J.C. Waerenborgh<sup>a</sup>, A. Amaro<sup>b</sup>, M. Godinho<sup>b</sup>, M. Almeida<sup>a</sup>

<sup>a</sup>*Departamento de Química, Instituto Tecnológico e Nuclear, Estrada Nacional 10, P-2686 Sacavém Codex, Portugal*

<sup>b</sup>*Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, Campo Grande ed. C1, P-1700 Lisboa, Portugal*

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### Abstract

A new uranium intermetallic compound, UFe<sub>2</sub>Zn<sub>20</sub>, was prepared and characterized by single-crystal X-ray diffraction, <sup>57</sup>Fe Mössbauer spectroscopy and magnetization measurements. It crystallizes in the cubic Fd $\bar{3}$ m space group ( $a=14.0998(9)$  Å) and is isostructural with CeCr<sub>2</sub>Al<sub>20</sub> ( $R=0.045$ ,  $W_{R2}=0.12$ ). Mössbauer spectra, taken between 5 K and room temperature, consist of a symmetric quadrupole doublet with narrow lines, confirming an ordered structure with the iron on only one crystallographic site and showing no magnetic ordering transition above 5 K, in good agreement with magnetization measurements. © 1998 Elsevier Science S.A.

**Keywords:** UFe<sub>2</sub>Zn<sub>20</sub>; Uranium compounds; Intermetallics

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### 1. Introduction

The existence of only two intermetallic compounds on the uranium–zinc system, U<sub>2</sub>Zn<sub>17</sub> and UZn<sub>12</sub>, has been firmly establish for a long time [1]. Both compounds present heavy-electron properties [2,3] and, aiming at the preparation of new intermetallics with interesting properties, we have started a systematic study of the U–Fe–Zn system. During this work a new low uranium content compound, UFe<sub>2</sub>Zn<sub>20</sub>, was found. In this paper we report its preparation and characterization by single-crystal X-ray diffraction, <sup>57</sup>Fe Mössbauer spectroscopy and preliminary magnetization data.

### 2. Experimental details

Small single crystals of a new U–Fe–Zn compound were grown in an sealed quartz tube by slowly cooling a (uranium+iron) solution in zinc. The starting composition of the solution was U:2Fe:100Zn. The mixture was heated under vacuum to 750°C, held at 750°C for 3 h and slow-cooled to 650°C. At this temperature the excess of liquid zinc was removed from the crystals by turning the ampoule upside down.

A small single crystal with approximate dimensions 0.12×0.14×0.10 mm<sup>3</sup> was transferred to a goniometer head on a Enraf-Nonius CAD-4 diffractometer with graphite monochromatized Mo K $\alpha$  radiation. The unit cell parameters were obtained by least-squares refinement of the  $2\theta$  values of 25 intense and well-centered reflections from various parts of the reciprocal space ( $16^\circ < 2\theta < 36^\circ$ ). The diffracted X-ray intensities were collected at room temperature using an  $\omega$ - $2\theta$  scan mode. The measured intensities were corrected for absorption by an empirical method based on  $\psi$  scans [4] and for Lorentz-polarization effects [5]. The structure was refined by full-matrix least-squares based on the squares of the structure factors [6].

Mössbauer absorbers, containing  $\approx 5$  mg of natural Fe cm<sup>-2</sup>, were prepared from powdered sample. Mössbauer spectra were measured in transmission mode using a conventional constant-acceleration spectrometer and a 25-mCi <sup>57</sup>Co source in a Rh matrix. The velocity scale was calibrated using an  $\alpha$ -Fe foil at room temperature. Spectra were obtained between 300 and 5 K. Low-temperature measurements were performed using a liquid-nitrogen/liquid helium flow cryostat. Mössbauer spectra were analysed using a modified version of the non-linear least-squares computer method of Stone and co-workers [7].

Magnetization measurements were performed in a single crystalline sample after zero field cooling and field cooling. The measurements were made in the 5–400 K temperature range and under fields up to 5 T applied

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\*Corresponding author. Tel.: +351 1 9550021; fax: +351 1 9941455; e-mail: apg@itn1.itn.pt

parallel to the *a*-axis using a SQUID magnetometer (Quantum Design MPMS).

### 3. Results and discussion

The cell parameters refinement revealed a cubic face-centered system (Space Group  $Fd\bar{3}m$ ) with  $a=14.0998(9)$  Å. Single-crystal X-ray diffraction data were refined to residuals  $R=0.045$  and  $R_w=0.120$  assuming a  $CeCr_2Al_{20}$ -type structure [8]. The final stage was performed considering that only Zn exists on the 48f and 96g sites. Site occupation factors of Fe and Zn on the 16c and 16d crystallographic positions were allowed to vary with the full site occupation as a constraint. 8a and 16d anisotropic temperature factors ( $U_{ij}$ ) had to be constrained to reasonable values (by analogy to those found by diffraction studies on similar compounds), otherwise they would converge to negative values. The final atomic parameters are summarized in Table 1. The relevant feature is that, within the experimental error, the uranium and iron atoms are located in only one crystallographic position (8a and 16d, respectively) and are surrounded exclusively by zinc atoms. Zinc atoms fully occupy the 16c, 48f and 96g crystallographic sites. A very small fraction of zinc in the 16d position can be eventually ruled out (0.3(2)). The final stoichiometry deduced from the X-ray diffraction refinement is consistent with a  $UFe_2Zn_{20}$  composition, and the small uncertainty results mainly from poor absorption corrections.

The 300 and 5 K Mössbauer spectra are presented in Fig. 1, and Table 2 contains estimated  $^{57}Fe$  Mössbauer parameters. In the temperature range 300–5 K, Mössbauer spectra may be fitted by a single narrow line width quadrupole splitting, in good agreement with the presence of iron in only one crystallographic position, as derived from the single-crystal X-ray structure. No magnetic ordering is observed down to 5 K. The estimated isomer shifts may seem large for iron in an intermetallic. They are, however, comparable to those found for iron impurities in metallic zinc [9].

The temperature dependence of the magnetization in a field of 10 000 Oe is shown in Fig. 2. The magnetization

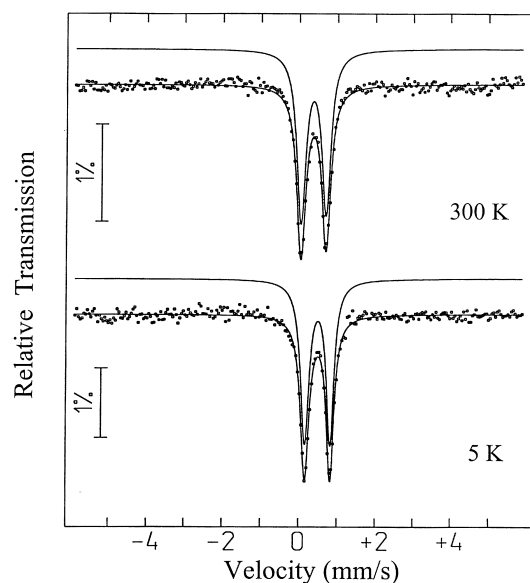


Fig. 1.  $^{57}Fe$  Mössbauer spectra of  $UFe_2Zn_{20}$  obtained at different temperatures.

Table 2

Estimated parameters from Mössbauer spectra of  $UFe_2Zn_{20}$  taken at 300 and 5 K

<i>T</i> (K)	$\delta$ (mm s <sup>-1</sup> )	$\Delta$ (mm s <sup>-1</sup> )	$\Gamma$ (mm s <sup>-1</sup> )
300	0.418(3)	0.657(4)	0.29(1)
5	0.536(3)	0.663(5)	0.28(1)

$\delta$ , isomer shift relative to metallic iron at room temperature;  $\Delta$ , quadrupole splitting;  $\Gamma$ , full width at half-maximum.

results confirm that from the Mössbauer effect. No magnetic transitions are seen down to 5 K, the magnetization increasing monotonically with decreasing temperatures.

### 4. Conclusions

In conclusion, a new uranium–iron–zinc intermetallic compound was prepared by high-temperature solution growth. This new compound presents a  $CeCr_2Al_{20}$ -type structure (cubic  $Fd\bar{3}m$  space group). In this structure the uranium and iron atoms are surrounded only by zinc. The

Table 1

Final results of the single-crystal XRD structural refinement of  $UFe_2Zn_{20}$

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	$U_{11}$	$U_{12}$	$U_{13}$	$U_{22}$	$U_{23}$	$U_{33}$	$U_{eq}$	s.o.f.
U	8a	1/8	1/8	1/8	0.10	0.10	0.10	0	0	0	—	1
Zn	16c	0	0	0	1.10(9)	1.10(9)	1.10(9)	−0.48(6)	−0.48(6)	−0.48(6)	1.11(9)	1.8(2)
Fe	16c	0	0	0	1.10(9)	1.10(9)	1.10(9)	−0.48(6)	−0.48(6)	−0.48(6)	1.11(9)	0.2(2)
Zn	16d	1/2	1/2	1/2	0.10 <sup>a</sup>	0.10 <sup>a</sup>	0.10 <sup>a</sup>	−0.04(5)	−0.04(5)	−0.04(5)	0.10	0.3(2)
Fe	16d	1/2	1/2	1/2	0.10 <sup>a</sup>	0.10 <sup>a</sup>	0.10 <sup>a</sup>	−0.04(5)	−0.04(5)	−0.04(5)	0.10	1.7(2)
Zn	48f	0.4893(1)	1/8	1/8	0.22(6)	0.17(4)	0.17(4)	−0.026(5)	0	0	0.19(4)	6
Zn	96g	0.0591(1)	0.0591(1)	0.3262(1)	0.72(4)	0.72(4)	0.26(5)	−0.04(2)	−0.04(2)	−0.39(4)	0.57(3)	12

<sup>a</sup>Equivalent isotropic temperature factor'  $U_{eq} = \frac{1}{3} \sum_{i=1}^3 \sum_{j=1}^3 U_{ij} a_i^* a_j^* a_i a_j$ .

<sup>b</sup>Fixed during refinement.

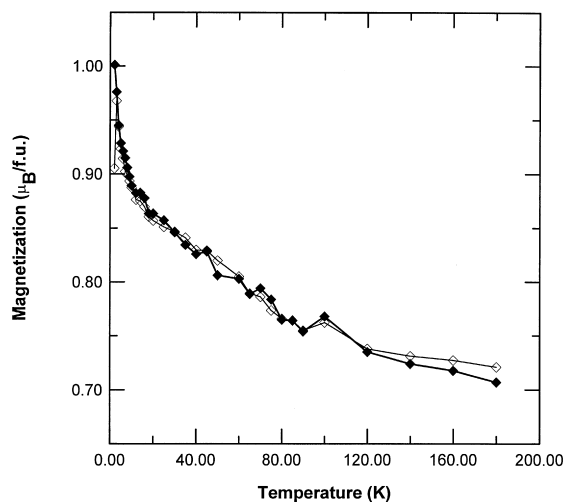


Fig. 2. Magnetization of the  $\text{UFe}_2\text{Zn}_{20}$  single crystal along the  $a$ -axis and in a field of 10 000 Oe, as a function of temperature (open symbols, zero field-cooled measurements; closed symbols, field-cooled measurements).

magnetization and Mössbauer measurements indicate that there is no magnetic transition down to 5 K.

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