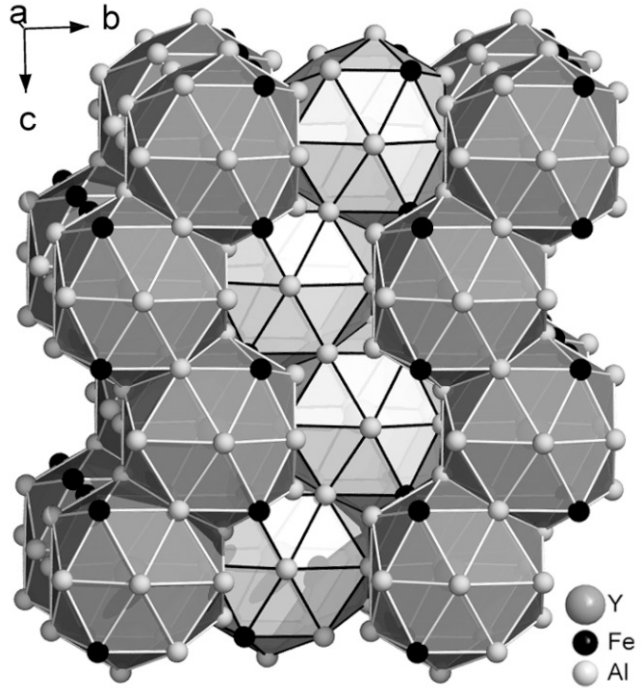
Crystal structure of yttrium iron aluminium (1/2/10), YFe_2Al_{10}

Alexander Kerkau[*, I], Liusuo Wu[II], Keesong Park[III], Yurii Prots[I], Manuel Brando[I], Meigan C. Aronson[II, III] and Guido Kreiner[I]

[I] Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany
[II] Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY 11794-3800, USA
[III] Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton NY 11973, USA

Received March 29, 2012, accepted June 12, 2012, available online August 09, 2012, CSD no. 710082



Abstract

YFe_2Al_{10}, orthorhombic, *Cmcm* (no. 63), a = 8.9654(2) Å, b = 10.1578(3) Å, c = 9.0110(3) Å, V = 820.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.018, $wR_{ref}(F^2)$ = 0.034, T = 295 K.

Table 1. Data collection and handling.

Crystal:	metallic blocks, size 0.050×0.055×0.065 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	114.89 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn724+ (2×2 bin mode), φ
$2\theta_{max}$:	66.9°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3585, 849
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 788
$N(param)_{refined}$:	40
Programs:	WinXPow [6], SHELX [7], DIAMOND [8]

Source of material

Singles crystals of YFe_2Al_{10} were grown from an aluminum flux with an initial molar composition of Y:Fe:Al=4:8:88. The metals purity of the elements (Alfa Aesar) is as follows: Yttrium (3N8, pieces), Iron (3N8, pieces) and Aluminum (5N, pieces). The elements and a Ta sieve were placed in a 5 cm^3 alumina crucible that was sealed in an evacuated quartz ampoule. The reaction mixture was heated to 1150 °C in four hours, and was kept at this temperature for additional four hours to homogenize the melt. After cooling to 960 °C within 90 hours it was placed in a centrifuge to remove the aluminum flux. Faceted, prismatic crystals of approximate 5x5x5 mm^3 size were found on the bottom of the alumina crucibles. Residual Al flux was removed mechanically.

* Correspondence author (e-mail: kerkau@cpfs.mpg.de)

Experimental details

The unit cell parameters were determined with the software WinXPow [6] from least-squares refinements of the 2θ values of 36 reflections (Cu Kα_1 radiation, λ = 1.54058 Å) in the range of 19° < 2θ < 100° using LaB_6 powder (NIST SRM660a, a = 4.1569(1) Å) as an internal standard. Metallographic examinations were carried out on a flat polished sample surface using optical and scanning electron microscopy. The investigations confirm that the sample is single phase material with some inclusions of elemental Al. The composition was checked by three EDXS measurements (50×50 μm, 15 kV, standardless ZAF correction) and corresponds to $Y_{0.98(1)}Fe_{2.04(3)}Al_{9.99(3)}$ (Y: 7.5(1) at.%, Fe: 15.7(2) at.%, Al: 76.8(2) at.%). Single crystal diffraction was carried out on a specimen mechanically separated from the large crystals.

Discussion

This study presents the crystal structure refinement of YFe_2Al_{10} based on single crystal diffraction data. YFe_2Al_{10} was first described by Jeitschko *et. al.* [1]. Crystallographic data based on Rietveld refinements of *X*-ray powder diffraction data was later provided by Waerenborgh *et. al.* [2]. YFe_2Al_{10} crystallizes with the $YbFe_2Al_{10}$ structure type which can be described as a combined substitution and stacking variant of the $ThMn_{12}$ and $CeMn_4Al_8$ type structures [3]. The coordination type polyhedron of Y is a Pseudo Frank-Kasper polyhedron CN20 ($12^{5.0}8^{6.0}$) with four Fe atoms at 3.416 Å, 14 Al atoms from 3.111 Å to 3.299 Å and two Al atoms at 3.646 Å distance. These polyhedra form zigzag chains along the [001] direction sharing common Al_4 rhombuses. The chains are arranged in the motif of a tetragonal rodlike packing [4] and are vertex connected by Al(1) atoms within the (001) plane. The Fe atoms are coordinated by 10 Al atoms at distances from 2.529 Å to 2.176 Å forming slightly distorted pentagonal antiprisms. Two additional Y atoms cap the pentagonal faces at 3.416 Å distance. Alternatively, the coordination of Fe can be described as a strongly distorted icosahedron ($12^{5.0}$). The five different types of Al atoms have irregular coordination type polyhedra with coordination numbers 12 for Al(1)/Al(5), 13 for Al(3) and 14 for Al(2)/Al(4). Each coordination polyhedron contains two Fe atoms, one or two Y atoms and between eight and eleven Al atoms. The shortest Al-Al distances of 2.576 Å are significantly smaller than observed in elemental Al (2.863 Å) [5].

Successive refinements of the site occupation factors of Fe and Al showed no significant deviation from the ideal composition.

Table 2. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Y(1)	4*c*	0	0.12663(3)	¼	0.0096(1)	0.0079(1)	0.0077(1)	0.0	0.0	0.0
Fe(1)	8*d*	¼	¼	0	0.0066(1)	0.0065(1)	0.0059(1)	0.00009(9)	–0.00051(9)	–0.0005(1)
Al(1)	8*g*	0.22621(7)	0.36128(6)	¼	0.0115(2)	0.0085(3)	0.0053(3)	0.0007(2)	0.0	0.0
Al(2)	8*g*	0.34899(6)	0.12877(6)	¼	0.0085(2)	0.0086(3)	0.0097(3)	–0.0008(2)	0.0	0.0
Al(3)	8*f*	0	0.15712(6)	0.59694(7)	0.0075(2)	0.0107(3)	0.0080(3)	0.0	0.0	0.0009(2)
Al(4)	8*f*	0	0.37536(6)	0.04856(8)	0.0079(2)	0.0086(3)	0.0131(3)	0.0	0.0	0.0015(2)
Al(5)	8*e*	0.22737(6)	0	0	0.0097(2)	0.0063(3)	0.0075(3)	0.0	0.0	0.0010(2)

Acknowledgments. The authors would like to thank Sylvia Kostmann, Petra Scheppan and Dr. Ulrich Burkhardt for metallographic examinations and EDXS measurements as well as Steffen Hückmann for collecting the powder diffraction data. Work at Brookhaven was carried out under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences under Contract no. DE-AC02-98CH1886.

References

1. Thiede, V.M.T.; Ebel, T.; Jeitschko, W.: Ternary aluminides LnT_2Al_{10} (Ln = Y, La-Nd, Sm, Gd-Lu and T = Fe, Ru, Os) with $YbFe_2Al_{10}$ type structure and magnetic properties of the iron-containing series. J. Mater. Chem. **8** (1998) 125-130.
2. Waerenborgh, J.C.; Salamakha, P.; Sologub, O.L.; Serio, S.; Godinho, M.; Goncalves, A.P.; Almeida, M.: Y-Fe-Al ternary system: partial isothermal section at 1070 K. Powder *X*-ray diffraction and Mössbauer spectroscopy study. J. Alloy. Compd. **323** (2001) 78-82.
3. Niemann, S.; Jeitschko, W.: The crystal structure of $YbFe_2Al_{10}$, a combined substitution and stacking variant of the $ThMn_{12}$ and $CeMn_4Al_8$ type structures. Z. Kristallogr. **210** (1995) 338-341.
4. O'Keeffe, M.; Andersson, S.: Rod packings and crystal chemistry. Acta Crystallogr. **A33** (1977) 914-923.
5. Donohue, Jerry: The structures of the elements, Wiley, New York (1974).
6. WinXPow Version 2.08, STOE & Cie GmbH, Darmstadt, Germany (2003).
7. Sheldrick, G.M.: A short history of SHELX. Acta Crystallogr. A64 (2008) 112-122.
8. Brandenburg, K. Putz, H. (2005). DIAMOND Version 3. Crystal Impact GbR, Postfach 1251, D-53002 Bonn, Germany.