Structural Heterogeneity in Twinned $Yb_{2-x}(Fe,Ga)_{17+2x}$ Polytypes

Y. Filinchuk[1], H. Birkedal[2, 3], R. Cerny[1], M. Hostettler[2], O. Bodak[4], K. Yvon[1]

Institut de Cristallographie

UNIVERSITÉ DE GENÈVE

[1] Laboratoire de Cristallographie, Universite de Genève, quai Ernest-Ansermet 24, CH-1211 Genève, Switzerland
[2] Institut de Cristallographie, Universite de Lausanne, BSP-Dorigny, CH-1015 Lausanne, Switzerland
[3] Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106, USA
[4] Ivan Franko National University of L'viv, 79005 L'viv, Kyryla&Mefodia 6, Ukraine

Sample preparation

The alloy was prepared by arc-melting at the nominal composition $Yb_{12}Fe_{64}Ga_{24}$

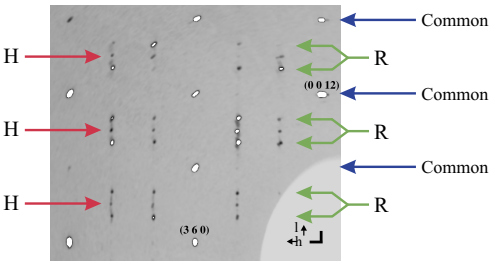
The ferromagnetic title compounds are substitution derivatives of R_2Fe_{17} (R = Rare earth) in which R and Fe atoms are partially substituted by Fe_2 dumbbells and Al(Ga) atoms, respectively.

According to previous work they crystallize with the hexagonal $LuFe_{0.5}$ type (1, $P6_3/mmc$) and/or rhombohedral $PrFe_7$ type (2, R-3m) structure. 1 and 2 (ABABAB and ABCABCABC stacking sequences) can be considered as polytypes with maximum degree of order (MDO polytypes).

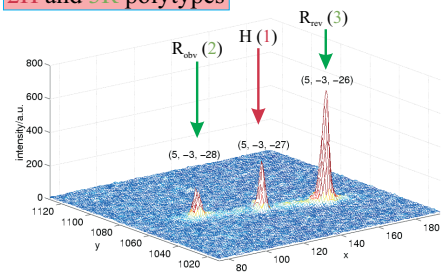
They have the cell parameter relationships $a(I) = a(II)$ and $3c(1) = 2c(2)$.

In this work we show that both polytypes can occur within a **coherently twinned crystal**.

h 2h l reciprocal space section of the "common cell"



2H and 3R polytypes



Structure investigations

Crystals of the cast sample showed peculiar non-space group absences and cell metrics $a(1) = a(2) = 8.615$ A and $3c(1) = 2c(2) = 25.215$ A.

Diffraction patterns: image plate detector, synchrotron radiation

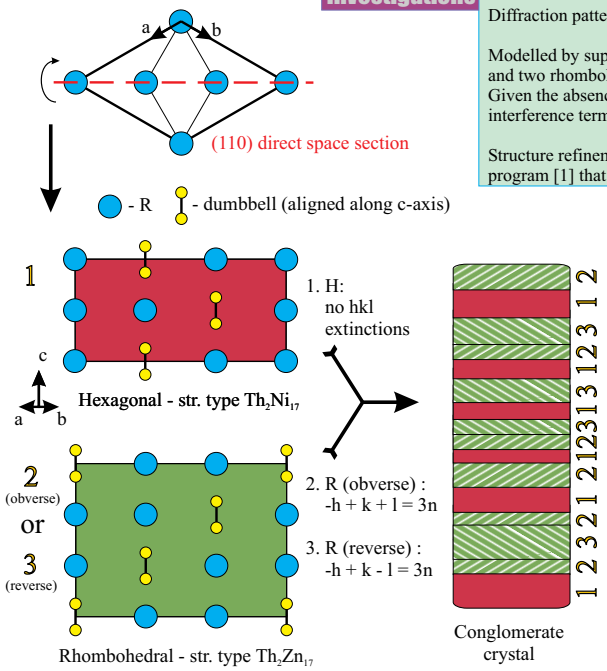
Modelled by superposing three sorts of domains: one hexagonal (1) and two rhombohedral (2, 3 - twinned by reticular merohedry). Given the absence of a significant diffuse scattering intensity interference terms arising from possible stacking-faults were neglected.

Structure refinement was performed by a newly developed computer program [1] that allows to refine several structures on a single data set.

Results

1 and 2(3) displayed different chemical compositions: 1 showed a higher rate of Yb substitution by Fe_2 dumbbells than 2(3), and 2(3) showed partial substitution of Fe by Ga.

Nano-scale chemically heterogeneous domains of the same crystal were structurally characterized for the first time.

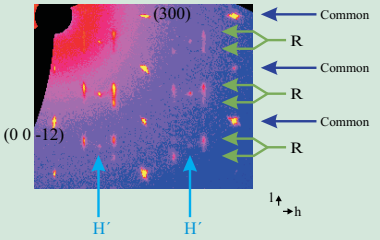


Diffuse intensity

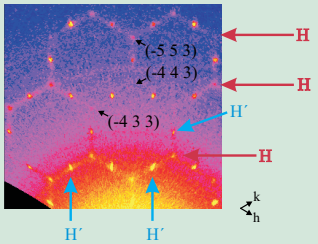
its amount in the streaks along c^* enabled us to find out the average domain size along c: evaluated qualitatively at the level of a few tens of unit cell dimensions

A crystal from an $Yb_{12}Fe_{65}Al_{23}$ alloy has the same structural features but shows an extra scattering (H´), with diffuse streaks in the basal plane. It suggests short-range order in it. Diffuse streaks for the reflections from R (2 and 3) domains indicate frequent stacking faults along c.

h 0 2l reciprocal space section of the "common cell"



h+k/2 k/2 3 reciprocal space section of the "common cell"



R: peaks of rhombohedral domains 2 and 3 are diffuse along c* direction

H: peaks of hexagonal domain 1 are not diffuse along a* or b*

H´: peaks can be indexed in H´(4) cell with a = 2a(1) =2a(2) and c = c(1) they have no diffuse streaks along c*

H´: peaks can be indexed in H´(4) cell with a = 2a(1) =2a(2) and c = c(1) they have diffuse streaks along a* and b*

evidence for local R-atom ordering in the basal plane different from that observed in Th_2Ni_{17} and Th_2Zn_{17} type structures

Data acquisition: ESRF (SNBL) λ = 0.55091 Å; crystal selected from a $Yb_{12}Fe_{64}Ga_{24}$ bulk

	the whole conglomerate		domain type 1		domain type 2		domain type 3	
crystal class			hexagonal		rhombohedral		rhombohedral	
space group			$P6_3/mmc$		$R\bar{3}m$		$R\bar{3}m$	
a (a_s = 8.615 Å)	a_s		a_s		a_s		a_s	
c (c_s = 25.215 Å)	c_s		$c_s/3$		$c_s/2$		$c_s/2$	
refined composition			$Yb_{3.46(2)}Fe_{35.07(4)}$		$Yb_{5.006(2)}Fe_{50.44(2)}Ga_{1.878(13)}$			
no. of parameters	41		18		20			
volume fraction			0.320(4)		0.340(3)		0.340(3)	
group of reflections	all	common	all	own	all	own	all	own
$R_1(F^2_o>3s(F^2_o))$	0.0644	0.0551	0.0635	0.0839	0.0597	0.0660	0.0591	0.0646
wR_2(all)	0.1857	0.1553	0.2102	0.2700	0.1625	0.1679	0.1626	0.1680
Goof(all)	1.0084							

Related topics:

1. What is a real $TbCu_7$ structure? Isn't it a highly disordered stacking of the layers that have a strong tendency to ordering in the basal plane?
2. D.S. Yufit *et al.* (2002). Acta Cryst., **B58**, 673-676 - two polytypes of organic substance in a coherently twinned crystal
3. H. Katzke. (2002). Z. Kristallogr., **217**, 127-130 - variations of peak profiles for 2H&3R twinned polytypes of NbS_2
4. D.L. Smith *et al.* (1981). Acta Cryst., **B37**, 1807-1812 - 2H&3R coherently twinned polytypes of CuNCS were refined

[1] H. Birkedal, M. Hostettler, W. Paciorek, D. Schwarzenbach, Bulletin of the Czech and Slovak Crystallographic Association. Special issue B, ECM-18 posters - abstracts. 5 (1998), 200 (Abstract A4-P17).