X-RAY POWDER DIFFRACTION DATA AND STRUCTURE REFINEMENT OF COMPOUND ErNi₂Si₂^①

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ABSTRACT The X-ray powder diffraction data for $ErNi_2Si_2$ are given and the crystal structure has been refined by the Rietveld whole pattern fitting method. The compound $ErNi_2Si_2$ crystallizes with the $ThCr_2Si_2$ type structure (tetragonal, space group I4/mmm, Z=2). The refined lattice parameters are a=3.9321(1) Å c=9.5237(1) Å and the structure was refined to $R_p=13.09\%$, $R_{wp}=16.69\%$. The figure of merit F_N for the powder data is $F_{30}=108.2$ (0.0063,44).

Key words ErNi₂Si₂ X-ray powder diffraction Rietveld structure refinement

1 INTRODUCTION

The rare earth compounds RET₂Si₂, where RE is a rare earth element and T is a transition metal element, have been studied with great interest for a few decades^[1]. Most of these compounds with ThCr₂Si₂ type structure (space group I4/mmm, standardized atom coordinates Th in 2a: 0, 0, 0; Cr in 4d: 0, 1/2, 1/4 and 1/2, 0, 1/4; Si in 4e: 0, 0, Z and 0, 0, -Z) have a variety of magnetic properties^[2, 3]. The crystal structure and X-ray powder diffraction data of a single phase are the basis of materials science study. Since there are no reports on Xray powder diffraction data for ErNi₂Si₂ in the Powder Diffraction File (PDF), in this paper, we report the X-ray powder diffraction data and the Rietveld structure refinement of ErNi₂Si₂.

2 EXPERIMENTAL

The sample of compound ErNi₂Si₂ was prepared by arc melting starting materials of at least 99.9% purity. The sample was turned upside down and remelted five times to ensure homo-

geneity. The mass loss of the sample during arc melting was less than 0.5%. To achieve equilibrium, the sample was wrapped with Ta foil, sealed into an evacuated quartz tube and annealed for 10 days at 1000 °C, then cooled at a rate of 10 °C/h to room temperature. The composition of the sample was confirmed by electron probe microanalysis (EPMA). The powder sample was obtained by pestling the annealed alloy to a particle size of less than 10 μ m in an agate mortar. The powder was sealed in an evacuated glass tube and annealed at 500 °C for 5 days, then cooled at a rate of 10 °C/h to room temperature.

Powder was loaded into aluminum cavity specimen holder by the "Rear loading sample preparation technique" proposed by Schreiner [4]. The X-ray powder diffraction experiment was performed for ErNi₂Si₂ on the Rigaku D/max-RC diffractometer equipped with a graphite monochromater using Cu K_{α} radiation (λ = 1.54060 Å). Data were collected in the stepscan mode with a step size of 0.02°(2 θ) and a counting time of 2s per step over the range of 15 ~ 140°(2 θ). Powder data were collected at room temperature (25 ± 1 °C). High purity Si powder was used as an internal standard for the

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determination of d value. Some of the experiment details are the same as that in Ref. [5]. The structure refinement of the compound $ErNi_2Si_2$ was carried out by the Rietveld whole pattern fitting method using the program DB-WS-9411PC^[7].

3 RESULTS AND DISCUSSION

3. 1 The X-ray powder diffraction data of ErNi₂Si₂

The XRD patterns of the sample consist of 88.51% (mass) $ErNi_2Si_2$ phase and 11.49% (mass) Er_2O_3 phase. The diffraction pattern was successfully indexed with a tetragonal lattice using the program $TREOR^{[\,8]}$ after excluding the peaks of Er_2O_3 . X-ray powder diffraction data for $ErNi_2Si_2$ are listed in Table 1. The Smith and Snyder figure of merit $^{[\,9]}$ $F_{\,30}$ is 108.2 (0.0063, 44), showing the powder pattern indexing is highly reliable.

Table 1 X-ray powder diffraction data for ErNi₂Si₂

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1		1ac	ne i	X-ray p	ow der di	iiraction (data 1	or ErN 125) 12		
24. 463 45 3. 636 101 3. 635 0. 006 32. 175 9 2. 780 110 2. 781 0. 009 36. 335 77 2. 471 103 2. 471 0. 001 37. 424 100 2. 401 112 2. 401 0. 005 37. 737 24 2. 382 004 2. 382 0. 004 2. 382 0. 004 14. 1808 1. 966 1. 729 5 211 1. 729 4 0. 005 0			$d_{ m obs}$ / Å	hkl	$d_{ m cal}$ / $ extstyle extsty$	Δ2 θ/ (°)	2 θ _{obs} / (°)		$d_{ m obs}$ /	hkl	$d_{ m cal}$ / $\mathring{\sf A}$	Δ2 θ/ (°)
32.175 9 2.780 110 2.781 0.009 36.335 77 2.471 103 2.471 0.001 96.620 6 1.0315 323 1.0315 0.003 1.0221 37.737 24 2.382 004 2.382 0.004 2.382 0.004 1.9662 0.001 103.158 5 0.98319 400 0.98310 0.014 103.772 7 0.97905 316 0.97901 0.006 1.0315 1.0315 1.0315 0.98310 0.014 1.03.772 7 0.97905 316 0.97901 0.006 0.96275 0.001 0.95263 0.001 0.95263 0.001 0.055263 0.001 0.005 0.0	18. 605	2	4. 765	002	4. 763	- 0.008	91.009	5	1.0800	305	1.0799	0.002
36, 335 77 2, 471 103 2, 471 0, 001 96, 620 6 1, 031 5 323 1, 031 5 - 0, 003 37, 424 100 2, 401 112 2, 401 0, 005 109 1, 022 1 109 1, 022 1 1, 018 5 - 0, 002 1, 018 5 - 0, 002 1, 018 5 - 0, 002 1, 018 6 208 1, 018 5 - 0, 002	24. 463	45	3.636	101	3. 635	- 0.006	91.402	6	1.0763	217	1.0763	0.002
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103.772 7	37.737	24	2. 382	004	2. 382	- 0.004	98. 267	10	1.0186	208	1.0185	- 0.002
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90.630 2 1.0834 321 1.0836 0.015		2					131. 227	3	0. 845 76	1011	0. 845 79	0.010
	90.630	2	1. 083 4	321	1.0836	0.015						

3. 2 Structure refinement of ErNi₂Si₂

The Rietveld method was used to refine the crystal structure of ErNi₂Si₂. The ErNi₂Si₂ phase and an impurity phase of Er₂O₃ were included in the refinement. The profile function used for describing the peak shape was a Pearson VII type, the background was modeled as a refined polynomial. The tetragonal ThCr₂Si₂ structure^[1] was used as a trial structure, and scattering factors were taken from International Tables for X-ray Crystallography^[10].

A total of 37 parameters, including 3 polynomial background and 20 structural parameters for ErNi₂Si₂ and 14 parameters for Er₂O₃ and for the global parameters of zero point, scale factor, preferred orientation and peak shape were refined.

The observed, calculated and difference diffraction patterns for the Rietveld refinement of ErNi₂Si₂ are displayed in Fig. 1.

The refined structural parameters and R factors of $ErNi_2Si_2$ are given in Table 2. The refined lattice parameters are a=3.9321(1) Å and c=9.5237(1) Å These results confirm that the compound $ErNi_2Si_2$ belongs to the tetragonal

ThCr₂Si₂ type structure with space group I4/mmm. Each unit cell contains two chemical formula units of ErNi₂Si₂. The pattern R factor $R_{\rm p}$ and the weighted pattern R factor $R_{\rm wp}$ obtained with the Rietveld refinement for ErNi₂Si₂ are 13.09% and 16.69%, respectively. Fig. 2 is a representation of the crystal structure of ErNi₂Si₂ in three dimensional view and the interatomic distances for ErNi₂Si₂ are given in Table 3.

Table 2 Refined atomic position parameters of ErNi₂Si₂

Atom	Site	x	у	z	N
\mathbf{Er}	2a	0	0	0	2. 0
Ni	4d	0	0.5	0.25	4. 0
Si	4e	0	0	0. 378 3(4)	4. 0

(ErNi₂Si₂: I/4mmm, No. 139; a = 3.9321(1) Å, c = 9.5237(1) Å, Z = 2; $R_{wp} = 16.69\%$, $R_p = 13.09\%$)

4 CONCLUSION

The X-ray powder diffraction data of ErNi₂Si₂ compound have been investigated by

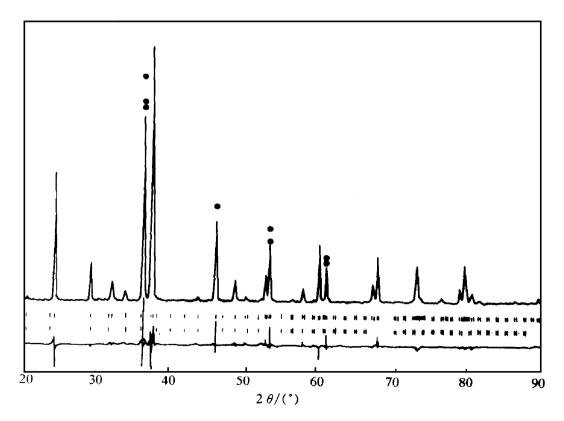


Fig. 1 The observed, calculated and difference diffraction patterns of ErNi₂Si₂

Table 3	Interatomic distances
fo	r ErNioSio(Å)

Atoms	Distance/ Å
Er-Er	3. 9321
Er-Ni	3. 0877
Er-Si	3. 0123
Nir S i	2. 3148
SrSi	2. 3181

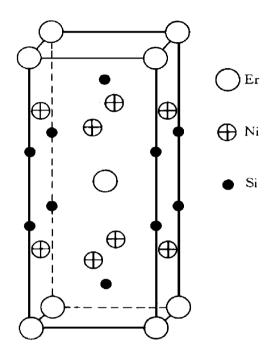


Fig. 2 The unit cell of ErNi₂Si₂ experimental methods and the crystal structure

has been refined by Rietveld method. The compound has the tetragonal ThCr₂Si₂ type structure, space group I4/mmm (No. 139), a = 3.9321(1) Å, c = 9.5237(1) Å, V = 147.249(3) Å³, Z = 2 and $D_x = 7.889 \text{g/cm}^3$. The refined results show that 2 Er, 4 Ni and 4 Si atoms occupy the 2a, 4d and 4e positions, respectively. The figure of merit F_N for the powder data is $F_{30} = 108.2(0.0063, 44)$.

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