# X-ray powder diffraction data for compound $Er_3Co_4Al_{12}$

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A new compound $Er_3Co_4Al_{12}$ was prepared by arc melting under argon atmosphere. The powder X-ray diffraction data of $Er_3Co_4Al_{12}$ were successfully indexed, giving a hexagonal structure with $a = 8.6185(2)$ Å, $c = 9.2347(3)$ Å, and unit-cell volume $V = 594.04$ Å$^3$. Compound $Er_3Co_4Al_{12}$ has the $Gd_3Ru_4Al_{12}$ type-structure, $Z = 2$ and space group $P6_3/mmc$. © *2013 International Centre for Diffraction Data.* [doi:10.1017/S0885715613000407]

Key words: erbium cobalt aluminum, powder X-ray diffraction

## I. INTRODUCTION

The RE–Co–Al (RE = rare earth) system is the basic system for the rare earth-based bulk metallic glasses, which have been the subject of recent intensive studies owing to their excellent glass forming ability, good mechanical and magnetic properties (Luo and Wang, 2009). A new compound $RE_3Co_4Al_{12}$ (RE = Dy, Er) was found during our investigation of the phase equilibria in the Er–Co–Al and Dy–Co–Al ternary systems. Analysis of the X-ray diffraction data of the compound showed that $RE_3Co_4Al_{12}$ has the hexagonal $Gd_3Ru_4Al_{12}$ type-structure, $Z = 2$, space group $P6_3/mmc$, isostructural with the compound $U_3Co_4Al_{12}$ (Tougait *et al.*, 2004). In this paper, the X-ray powder diffraction data up to 110°2$\theta$ of the new compound $Er_3Co_4Al_{12}$ are reported.

## II. EXPERIMENTAL

The sample was prepared by arc melting of Er (99.95%), Co (99.9%), and Al (99.99%) on a water-cooled copper hearth with a non-consumable tungsten electrode under argon atmosphere. The sample was turned and remelted three times to ensure sample homogeneity. The ingot obtained was annealed in an evacuated quartz tube at 600 °C for 600 h and then cooled down slowly to 500 °C, kept for 480 h before quenching in liquid nitrogen. Specimen for XRD measurements was ground in agate mortar and pestle to a particle size of less than 10 μm, loaded in Al well and gently pressed. Two sets of the powder XRD patterns, with or without Si added as an internal standard, were collected at room temperature on a Rigaku D/Max 2500 V diffractometer with Cu$K\alpha_1$ ($\lambda = 1.54060$ Å) and a graphite monochromator. The scan ranged from 10 to 110° 2$\theta$ with a step size of 0.02° and a counting time of 2 s per step. The XRD pattern recorded from the specimen added with high purity Si (99.999%) internal standard was used to obtain the observed peak positions $2\theta_{obs}$ for indexing, while the XRD pattern without Si internal standard was used for the observed peak height $I_{obs}$. The Jade software package (Materials Data, Inc., Livermore, California) was used to analyze the data. The $2\theta_{obs}$ values of the peaks were determined by the Savitzky–Golay second derivative method after background subtracting, $K\alpha_2$ stripping and Si internal standard calibration using PDF 027-1402 (ICDD, 2011) with $\lambda = 1.540598$ Å. Pattern indexing was performed using the program TREOR (Werner *et al.*, 1985) and the values of unit-cell parameters were obtained.

## III. RESULTS

The powder XRD pattern indicated that the trace amount of the impurity phase identified as $Er_2O_3$ (PDF 43-1007) (ICDD, 2011) was detected as well as $Er_3Co_4Al_{12}$. The strongest reflection of the $Er_2O_3$ phase did not overlap with those of $Er_3Co_4Al_{12}$ and its peak height is less than 3%. The experimental XRD pattern of compound $Er_3Co_4Al_{12}$ is shown in Figure 1. All lines except for those corresponding to $Er_2O_3$ were successfully indexed using TREOR and it showed that the compound $Er_3Co_4Al_{12}$ is hexagonal with unit-cell parameters $a = 8.6185(2)$ Å, $c = 9.2347(3)$ Å, and unit-cell volume $V = 594.04$ Å$^3$. The figure of merit for indexing $F_N$ (Smith and Snyder, 1979) is $F_{30} = 123.2$ (0.0058, 42). The X-ray powder diffraction data for $Er_3Co_4Al_{12}$ are listed in Table I. The peak height values of the calculated relative

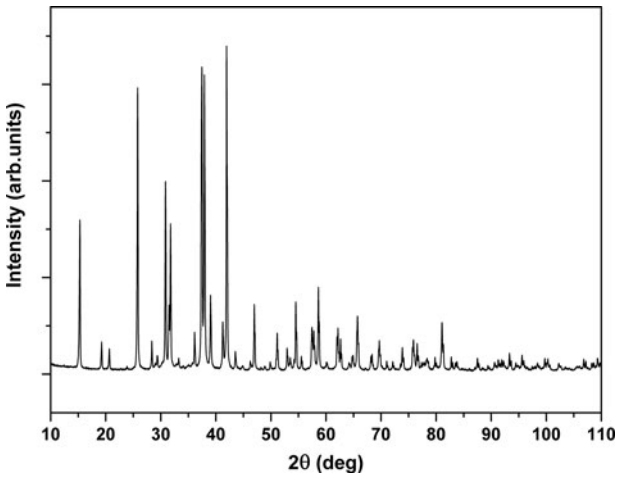


Figure 1. Powder diffraction pattern of $Er_3Co_4Al_{12}$ (Cu$K\alpha_1$ radiation, $\lambda = 1.54060$ Å, 40 kV, 150 mA, step size 0.02°, and counting time 1 s per step).

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TABLE I. X-ray powder diffraction data for $Er_3Co_4Al_{12}$ [$P6_3/mmc$, $a = 8.6185(2)$ Å, $c = 9.2347(3)$ Å, $V = 594.04$ Å$^3$, $Z = 2$, Cu$K\,\alpha_1$, and $\lambda = 1.54060$ Å]. Only those peaks with $I_{obs}$ of 1 or greater are presented.

| No. | $2\theta_{obs}$ (°) | $d_{obs}$ (Å) | $I_{obs}$ | $h$ | $k$ | $l$ | $2\theta_{cal}$ (°) | $d_{cal}$ (Å) | $I_{cal}$ | $\Delta 2\theta$ (°) |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 15.236 | 5.811 | 36 | 1 | 0 | 1 | 15.251 | 5.8049 | 52 | −0.015 |
| 2 | 19.196 | 4.620 | 7 | 0 | 0 | 2 | 19.207 | 4.6174 | 13 | −0.011 |
| 3 | 20.580 | 4.312 | 5 | 1 | 1 | 0 | 20.594 | 4.3093 | 3 | −0.014 |
| 4 | 23.825 | 3.732 | 1 | 2 | 0 | 0 | 23.824 | 3.7319 | 1 | 0.001 |
| 5 | 25.718 | 3.461 | 76 | 2 | 0 | 1 | 25.727 | 3.4601 | 80 | −0.009 |
| 6 | 28.310 | 3.150 | 8 | 1 | 1 | 2 | 28.306 | 3.1504 | 7 | 0.004 |
| 7 | 30.778 | 2.903 | 54 | 2 | 0 | 2 | 30.781 | 2.9024 | 59 | −0.003 |
| 8 | 31.402 | 2.846 | 17 | 1 | 0 | 3 | 31.410 | 2.8457 | 22 | −0.008 |
| 9 | 31.696 | 2.821 | 41 | 2 | 1 | 0 | 31.692 | 2.8211 | 36 | 0.004 |
| 10 | 33.181 | 2.698 | 2 | 2 | 1 | 1 | 33.179 | 2.6980 | 1 | 0.002 |
| 11 | 36.062 | 2.489 | 10 | 3 | 0 | 0 | 36.072 | 2.4879 | 10 | −0.010 |
| 12 | 37.341 | 2.406 | 79 | 2 | 1 | 2 | 37.324 | 2.4073 | 60 | 0.017 |
| 13 | 37.858 | 2.375 | 88 | 2 | 0 | 3 | 37.856 | 2.3747 | 100 | 0.002 |
| 14 | 38.995 | 2.308 | 22 | 0 | 0 | 4 | 38.981 | 2.3087 | 39 | 0.014 |
| 15 | 41.181 | 2.190 | 14 | 3 | 0 | 2 | 41.182 | 2.1902 | 18 | −0.001 |
| 16 | 41.898 | 2.154 | 100 | 2 | 2 | 0 | 41.895 | 2.1546 | 80 | 0.003 |
| 17 | 43.480 | 2.0797 | 5 | 2 | 1 | 3 | 43.478 | 2.0798 | 6 | 0.002 |
| 18 | 46.202 | 1.9633 | 3 | 2 | 0 | 4 | 46.200 | 1.9634 | 3 | 0.002 |
| 19 | 46.920 | 1.9349 | 21 | 3 | 0 | 3 | 46.918 | 1.9350 | 28 | 0.002 |
| 20 | 49.821 | 1.8288 | 3 | 4 | 0 | 1 | 49.816 | 1.8290 | 1 | 0.005 |
| 21 | 50.899 | 1.7926 | 4 | 1 | 0 | 5 | 50.890 | 1.7929 | 2 | 0.009 |
| 22 | 51.080 | 1.7867 | 11 | 2 | 1 | 4 | 51.080 | 1.7867 | 14 | 0.000 |
| 23 | 52.880 | 1.7300 | 7 | 4 | 0 | 2 | 52.879 | 1.7300 | 6 | 0.001 |
| 24 | 53.285 | 1.7178 | 2 | 3 | 1 | 3 | 53.285 | 1.7178 | 1 | 0.000 |
| 25 | 53.475 | 1.7121 | 3 | 3 | 2 | 0 | 53.469 | 1.7123 | 4 | 0.006 |
| 26 | 54.145 | 1.6925 | 3 | 3 | 0 | 4 | 54.152 | 1.6923 | 2 | −0.007 |
| 27 | 54.458 | 1.6835 | 22 | 3 | 2 | 1 | 54.455 | 1.6836 | 19 | 0.003 |
| 28 | 55.462 | 1.6554 | 4 | 2 | 0 | 5 | 55.466 | 1.6553 | 7 | −0.004 |
| 29 | 57.397 | 1.6041 | 13 | 4 | 1 | 1 | 57.402 | 1.6040 | 7 | −0.005 |
| 30 | 57.737 | 1.5955 | 12 | 4 | 0 | 3 | 57.729 | 1.5957 | 9 | 0.008 |
| 31 | 58.558 | 1.5751 | 26 | 2 | 2 | 4 | 58.552 | 1.5752 | 23 | 0.006 |
| 32 | 60.042 | 1.5396 | 2 | 0 | 0 | 6 | 60.064 | 1.5391 | 3 | −0.022 |
| 33 | 61.960 | 1.4965 | 11 | 3 | 2 | 3 | 61.965 | 1.4964 | 16 | −0.005 |
| 34 | 62.120 | 1.4930 | 9 | 5 | 0 | 0 | 62.131 | 1.4928 | 8 | −0.011 |
| 35 | 62.582 | 1.4831 | 10 | 3 | 0 | 5 | 62.588 | 1.4830 | 12 | −0.006 |
| 36 | 64.179 | 1.4500 | 2 | 1 | 1 | 6 | 64.206 | 1.4494 | 2 | −0.027 |
| 37 | 64.700 | 1.4396 | 4 | 4 | 1 | 3 | 64.696 | 1.4396 | 3 | 0.004 |
| 38 | 64.842 | 1.4368 | 3 | 3 | 3 | 0 | 64.859 | 1.4364 | 4 | −0.017 |
| 39 | 65.562 | 1.4227 | 13 | 2 | 0 | 6 | 65.554 | 1.4229 | 10 | 0.008 |
| 40 | 65.680 | 1.4204 | 16 | 5 | 0 | 2 | 65.683 | 1.4204 | 17 | −0.003 |
| 41 | 68.135 | 1.3751 | 4 | 3 | 2 | 4 | 68.123 | 1.3753 | 7 | 0.012 |
| 42 | 68.322 | 1.3718 | 3 | 3 | 3 | 2 | 68.335 | 1.3716 | 5 | −0.013 |
| 43 | 69.538 | 1.3508 | 7 | 2 | 1 | 6 | 69.517 | 1.3511 | 9 | 0.021 |
| 44 | 69.638 | 1.3491 | 9 | 4 | 2 | 2 | 69.643 | 1.3490 | 6 | −0.005 |
| 45 | 70.981 | 1.3268 | 3 | 5 | 1 | 1 | 70.991 | 1.3266 | 4 | −0.010 |
| 46 | 72.099 | 1.3090 | 3 | 3 | 0 | 6 | 72.102 | 1.3089 | 5 | −0.003 |
| 47 | 73.515 | 1.2872 | 2 | 5 | 1 | 2 | 73.503 | 1.2874 | 1 | 0.012 |
| 48 | 73.823 | 1.2826 | 7 | 4 | 2 | 3 | 73.841 | 1.2823 | 5 | −0.018 |
| 49 | 75.680 | 1.2557 | 7 | 3 | 2 | 5 | 75.678 | 1.2557 | 6 | 0.002 |
| 50 | 75.821 | 1.2537 | 9 | 5 | 0 | 4 | 75.830 | 1.2536 | 8 | −0.009 |
| 51 | 76.519 | 1.2440 | 8 | 6 | 0 | 0 | 76.519 | 1.2440 | 4 | 0.000 |
| 52 | 77.302 | 1.2333 | 2 | 6 | 0 | 1 | 77.338 | 1.2328 | 2 | −0.036 |
| 53 | 77.760 | 1.2272 | 2 | 4 | 3 | 0 | 77.771 | 1.2270 | 2 | −0.011 |
| 54 | 78.199 | 1.2214 | 3 | 4 | 1 | 5 | 78.184 | 1.2216 | 2 | 0.015 |
| 55 | 79.761 | 1.2014 | 4 | 6 | 0 | 2 | 79.778 | 1.2011 | 5 | −0.017 |
| 56 | 80.922 | 1.1870 | 6 | 4 | 0 | 6 | 80.897 | 1.1873 | 3 | 0.025 |
| 57 | 81.040 | 1.1856 | 16 | 4 | 3 | 2 | 81.016 | 1.1859 | 5 | 0.024 |
| 58 | 82.723 | 1.1657 | 4 | 3 | 0 | 7 | 82.738 | 1.1655 | 5 | −0.015 |
| 59 | 83.481 | 1.1570 | 2 | 5 | 2 | 2 | 83.480 | 1.1570 | 2 | 0.001 |
| 60 | 83.796 | 1.1535 | 2 | 6 | 0 | 3 | 83.807 | 1.1534 | 2 | −0.011 |
| 61 | 87.480 | 1.1141 | 4 | 5 | 2 | 3 | 87.480 | 1.1141 | 4 | 0.000 |
| 62 | 89.365 | 1.0955 | 2 | 6 | 0 | 4 | 89.400 | 1.0951 | 1 | −0.035 |
| 63 | 90.603 | 1.0837 | 2 | 4 | 3 | 4 | 90.621 | 1.0835 | 2 | −0.018 |
| 64 | 91.282 | 1.0774 | 3 | 4 | 4 | 0 | 91.290 | 1.0773 | 2 | −0.008 |
| 65 | 91.939 | 1.0714 | 3 | 5 | 0 | 6 | 91.921 | 1.0716 | 5 | 0.018 |

*Continued*


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TABLE I. Continued

| No. | $2\theta_{obs}$ (°) | $d_{obs}$ (Å) | $I_{obs}$ | $h$ | $k$ | $l$ | $2\theta_{cal}$ (°) | $d_{cal}$ (Å) | $I_{cal}$ | $\Delta 2\theta$ (°) |
|---|---|---|---|---|---|---|---|---|---|---|
| 66 | 92.264 | 1.0685 | 2 | 2 | 1 | 8 | 92.276 | 1.0684 | 2 | −0.012 |
| 67 | 93.302 | 1.0593 | 5 | 7 | 0 | 1 | 93.309 | 1.0592 | 2 | −0.007 |
| 68 | 94.481 | 1.0492 | 2 | 4 | 4 | 2 | 94.483 | 1.0491 | 2 | −0.002 |
| 69 | 95.617 | 1.0397 | 5 | 4 | 2 | 6 | 95.591 | 1.0399 | 5 | 0.026 |
| 70 | 96.195 | 1.0350 | 1 | 6 | 2 | 0 | 96.184 | 1.0350 | 2 | 0.011 |
| 71 | 97.405 | 1.0253 | 1 | 4 | 1 | 7 | 97.424 | 1.0251 | 1 | −0.019 |
| 72 | 97.999 | 1.0207 | 1 | 6 | 1 | 4 | 97.969 | 1.0209 | 1 | 0.030 |
| 73 | 98.440 | 1.0173 | 2 | 2 | 2 | 8 | 98.408 | 1.0175 | 3 | 0.032 |
| 74 | 99.742 | 1.0075 | 4 | 7 | 0 | 3 | 99.732 | 1.0075 | 2 | 0.010 |
| 75 | 100.301 | 1.0033 | 4 | 5 | 2 | 5 | 100.293 | 1.0034 | 4 | 0.008 |
| 76 | 102.243 | 0.9895 | 2 | 2 | 0 | 9 | 102.262 | 0.9894 | 4 | −0.019 |
| 77 | 103.48 | 0.9810 | 1 | 6 | 2 | 3 | 103.471 | 0.9811 | 1 | 0.009 |
| 78 | 105.663 | 0.9667 | 1 | 7 | 1 | 2 | 105.658 | 0.9667 | 1 | 0.005 |
| 79 | 106.815 | 0.9594 | 4 | 4 | 3 | 6 | 106.807 | 0.9595 | 2 | 0.008 |
| 80 | 107.177 | 0.9572 | 1 | 3 | 2 | 8 | 107.178 | 0.9572 | 2 | −0.001 |
| 81 | 108.262 | 0.9506 | 2 | 5 | 4 | 1 | 108.261 | 0.9506 | 2 | 0.001 |
| 82 | 108.587 | 0.9486 | 2 | 3 | 0 | 9 | 108.596 | 0.9486 | 2 | −0.009 |
| 83 | 109.319 | 0.9443 | 4 | 6 | 2 | 4 | 109.291 | 0.9445 | 6 | 0.028 |

intensities $I_{cal}$ were obtained using the LAZY-PULVERIX program (Yvon K *et al.*, 1977) based on the structure of the compound $U_3Co_4Al_{12}$ (Tougait *et al.*, 2004). All reflections are consistent with the $P6_3/mmc$ space group.

## SUPPLEMENTARY MATERIALS AND METHODS

The Supplementary material referred to in this article can be found online at journals.cambridge.org/pdj.

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