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Crystal structures of some equi-atomic gadolinium compounds*.

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In a program dealing with the properties of 4*f* and 5*f* transition metals and alloys a number of equi-atomic alloys of gadolinium were prepared; specifically, they were GdAl, GdCu, GdRh, GdAg and GdAu. At the time this work was initiated the crystal structures of GdAl (Baenziger & Moriarty, 1961), GdCu (Dwight, 1959*a*; Baenziger & Moriarty, 1961) and GdAg (Dwight, 1959*b*; Iandelli, 1960; Baenziger & Moriarty, 1961) had been reported in the literature. Since then data have also been published for GdAu (Chao, Luo & Duwez, 1963). The results obtained in this study are in reasonable agreement with the previously published data, except for GdAl.

The alloys were prepared by arc-melting together weighed amounts of the two components. X-ray samples taken from the arc-cast buttons were sealed in evacuated Pyrex capillary tubes and heat treated for 15 min at 500 °C and then water quenched. The X-ray pattern of the GdRh sample obtained in this manner was quite poor. A second heat treatment of 15 min at 550 °C, however, was sufficient to provide sharp back-reflection doublets. The powder patterns were taken by using a 114·59 mm diameter Debye–Scherrer camera and filtered copper radiation. The lattice constants for the b.c.c., CsCl type compounds of GdCu, GdRh and GdAg were calculated from $K\alpha_1$ and $K\alpha_2$ doublets in the back-reflection region by using a φ tan φ extrapolation method. For GdAl and GdAu the lattice constants were obtained by the Nelson–Riley extrapolation method.

The X-ray patterns of GdCu, GdRh and GdAg were easily indexed as b.c.c., CsCl, *B*2 type compounds and contained no extra lines. The lattice parameters of these compounds, which were corrected for refraction, are summarized in Table 1. The powder patterns of GdAl and GdAu were quite complex, which is in agreement with previous data. In the case of GdAl the lines for the b.c.c. phase reported by Baenziger & Moriarty (1961) could not be identified in the powder pattern. For GdAu, however, it was possible to identify most of the b.c.c., CsCl type lines in the complex pattern, which is in accord with the results of Chao, Luo & Duwez (1963). The non-cubic phase in both the GdAl and GdAu powder patterns was indexed as having an orthorhombic structure. These results are discussed below and the lattice parameters are summarized in Table 1.

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Table 1. *Lattice parameters and structural data for some* GdM *compounds, where* M *is* Al, Cu, Rh, Ag *or* Au

Compound	Lattice constant	Structure type	Reference
GdAl	$a = 3{\cdot}7208 \pm 0{\cdot}0002$ Å	CsCl + 2nd phase	(*a*)
GdAl	$a = 9{\cdot}274 \pm 0{\cdot}007$ $b = 7{\cdot}679 \pm 0{\cdot}008$ $c = 5{\cdot}584 \pm 0{\cdot}003$	CeAl	This paper
GdCu	$a = 3{\cdot}505$	CsCl	(*b*)
GdCu	$a = 3{\cdot}503 \pm 0{\cdot}001$	CsCl	(*a*)
GdCu	$a = 3{\cdot}5020 \pm 0{\cdot}0004$	CsCl	This paper
GdRh	$a = 3{\cdot}4425 \pm 0{\cdot}0006$	CsCl	This paper
GdAg	$a = 3{\cdot}66$	CsCl	(*c*)
GdAg	$a = 3{\cdot}653$	CsCl	(*d*)
GdAg	$a = 3{\cdot}6476 \pm 0{\cdot}0008$	CsCl	(*a*)
GdAg	$a = 3{\cdot}6491 \pm 0{\cdot}0002$	CsCl	This paper
GdAu	$a = 3{\cdot}593 \pm 0{\cdot}002$	CsCl + 2nd phase	(*e*)
GdAu	$a = 3{\cdot}6009 \pm 0{\cdot}0008$ $a = 4{\cdot}522 \pm 0{\cdot}005$ $b = 10{\cdot}826 \pm 0{\cdot}008$ $c = 4{\cdot}734 \pm 0{\cdot}004$	CsCl and CrB	This paper This paper

(*a*) Baenziger & Moriarty (1961). (*b*) Dwight (1959*a*). (*c*) Dwight (1959*b*). (*d*) Iandelli (1960). (*e*) Chao, Luo & Duwez (1963).

Examination of the published literature indicates that the rare earth-aluminum compounds, RAl, crystallize with either b.c.c., CsCl type or one of two different orthorhombic structures, *i.e.* CeAl type, which belongs to the space group $Cmc2_1$ (van Vucht, 1957) or CrB type found for YAl (Dagerhamn, 1963). All the lines in the GdAl powder pattern could be indexed on the basis of the CeAl type orthorhombic structure. Although Baenziger & Moriarty (1961) found some b.c.c. lines in their complex X-ray pattern for GdAl while none were found in this research, this does not necessarily indicate that one of the results is incorrect. The difference could be explained by the existence of a high-temperature b.c.c. phase retained upon quenching by Baenziger & Moriarty (1961) but not retained in this research because of either too slow a cooling rate during quenching or too low an annealing temperature, *i.e.* below the orthorhombic $\rightleftarrows$ b.c.c. transition temperature.

Chao, Luo & Duwez (1963) found that when GdAu was very rapidly quenched, only the b.c.c. lines were observed, but when this compound was slowly cooled both the complex and b.c.c. lines were obtained. No other literature data are available concerning the structures of the complex phase of any of the rare-earth-gold equi-atomic compounds. All the lines, other than those which were indexed as b.c.c., CsCl type, could be indexed as orthorhombic CrB, B_f type.

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