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NEUTRON DIFFRACTION STUDY OF THE Ho-Fe SYSTEM

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Résumé. — Les propriétés magnétiques des composés intermétalliques dans le système Ho-Fe ont été étudiées. Une analyse par diffraction neutronique sur un grand nombre de raies magnétiques a été entreprise sur HoFe_2 , $\text{Ho}_6\text{Fe}_{23}$ et $\text{Ho}_2\text{Fe}_{17}$. Les valeurs des moments magnétiques localisés sur les atomes de fer ont été trouvées indépendantes de la concentration en terre rare dans ces alliages, contrairement à ce qui a été trouvé précédemment pour le cobalt et le nickel dans les composés intermétalliques de même type. Les valeurs des moments de Ho et Fe sont en bon accord avec les aimantations spontanées mesurées en supposant un arrangement antiparallèle des moments de Ho et Fe. Les températures de Curie sont respectivement pour ces trois composés, de 610 °K, 560 °K et 325 °K ; leur décroissance, lorsque la concentration en fer augmente est analysée en fonction des nombres de coordination et des distances interatomiques entre atomes de fer, selon la théorie de Néel-Slater.

Abstract. — The magnetic properties of intermetallic compounds in the Ho-Fe system have been investigated. Neutron diffraction analyses have been carried out on HoFe_2 , $\text{Ho}_6\text{Fe}_{23}$ and $\text{Ho}_2\text{Fe}_{17}$ over a large range of magnetic reflections. The magnetic moments of the Fe atoms are found to be localized and not dependent on the rare earth amount in the alloys as has been found previously in Co or Ni intermetallic compounds. The moment values of Ho and Fe are in good agreement with the measured spontaneous magnetization assuming a ferrimagnetic model. The decrease of Curie temperature, 610 °K, 560 °K and 325 °K respectively, with increasing iron concentration is discussed in terms of coordination number and interatomic distances between the Fe atoms, according to the Néel-Slater theory.

I. Introduction. — Numerous investigations on the magnetic properties of binary alloys in the rare earth-cobalt and rare earth-nickel systems have shown a ferrimagnetic coupling between the rare earth moments and the magnetic moments localized on the transition metal elements. Moreover a decrease of the Curie temperature has been found to correspond to a decrease of the amount of the transition element in the alloy ; an important variation of the Co and Ni moments relative to the type and concentration of the rare earth alloy has been determined. This study of the (Ho-Fe) system has revealed the same type of uniaxial ferrimagnetic coupling between the rare earth and Fe moments but an increase of the Curie temperature has been found to correspond to a decrease of the concentration of the transition element. This significantly different behaviour of the compounds in the (Ho-Fe) system which has been found in the other R-Fe series suggested the need of an accurate neutron diffraction analysis to determine the type of exchange interaction existing between the magnetic moments.

II. Preparation. — Crystal Structure. — The phase diagram of the (Ho-Fe) system has been studied by Roe et al. [1]. The compounds HoFe_2 , HoFe_3 , $\text{Ho}_6\text{Fe}_{23}$ and $\text{Ho}_2\text{Fe}_{17}$ have been identified. The crystal structure of HoFe_2 is isomorphous with the cubic MgCu_2 , [2] Laves phase. HoFe_3 has the rhombohedral PuNi_3 [3] structure ; the cubic $\text{Ho}_6\text{Fe}_{23}$ is of the $\text{Th}_6\text{Mn}_{23}$ [4] type and the hexagonal $\text{Ho}_2\text{Fe}_{17}$ is of the $\text{Th}_2\text{Ni}_{17}$ [5] type. The lattice parameters are reported in Table I.

TABLE I

Lattice Parameters of Ho-Fe Compounds

	HoFe_2	HoFe_3	$\text{Ho}_6\text{Fe}_{23}$	$\text{Ho}_2\text{Fe}_{17}$
System	Cubic	Hexagonal	Cubic	Hexagonal
Parameters (Å)	$a = 7.305$	$a = 5.084$ $c = 24.45$	$a = 12.032$	$a = 8.438$ $c = 8.310$

III. Magnetic Measurements. — A thermomagnetic investigation of HoFe_2 , HoFe_{23} and $\text{Ho}_2\text{Fe}_{17}$ has shown a ferrimagnetic behavior of these compounds. The absolute saturation magnetization values, extrapolated to 0 °K, suggested a ferrimagnetic coupling between the Ho and Fe sublattices. The Curie temperatures are listed in Table II.

TABLE II

Curie Temperatures of Ho-Fe Compounds

	HoFe_2	HoFe_3	$\text{Ho}_6\text{Fe}_{23}$	$\text{Ho}_2\text{Fe}_{17}$
T_c (°K)	610	580	560	325

The uniaxial configuration of the magnetic moments of HoFe_2 and $\text{Ho}_2\text{Fe}_{17}$ has been determined on powder samples lined up in a magnetic field of approximately 5 kOe. The easy direction of magnetization has been determined as [100] for HoFe_2 in agreement with Mössbauer studies, Bowden [6] and in the basal plane for $\text{Ho}_2\text{Fe}_{17}$ at room temperature. Debye Scherrer diagrams for HoFe_2 before and after alignment in a magnetic field are shown in figure 1.

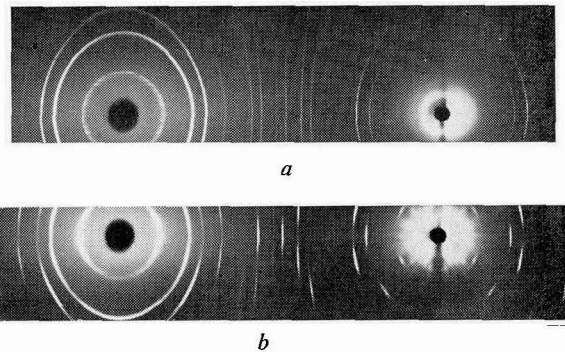


FIG. 1. — Debye Scherrer diagrams of HoFe_2 (a) before alignment in magnetic field and (b) after alignment in magnetic field.

IV. Neutron diffraction Analysis. Discussion. — Neutron diffraction analysis has been carried out at the Oak Ridge National Lab. Research Reactor on HoFe_2 , $\text{Ho}_6\text{Fe}_{23}$ and $\text{Ho}_2\text{Fe}_{17}$. The calculated and observed magnetic intensities of $\text{Ho}_2\text{Fe}_{17}$ are given in Table III.

TABLE III
Magnetic Intensities of $\text{Ho}_2\text{Fe}_{17}$
at Liquid Nitrogen Temperature

hkl	$I_{\text{obs.}}$	I_c	hkl	$I_{\text{obs.}}$	I_c
001	0.0	0.0	122	6.55	5.13
100	34.94	29.76	203	7.76	3.24
101	124.02	109.13	220	19.11	16.09
110	313.50	318.18	302	26.53	24.62
002	581.14	585.76	004	7.29	0.46
111	0.0	0.0	221	0.0	0.0
200	13.85	10.86	310	16.45	18.50
102	20.48	16.11	104	8.38	7.59
201	49.05	47.35	131	47.87	53.00
112	276.40	261.70	123	17.09	14.77
003	0.0	0.0	222	475.79	462.41
210	13.38	14.21	114	483.49	499.61
202	6.16	6.07	303	0.0	0.0
121	39.32	40.66	400	18.28	19.56
103	42.10	40.06	132	9.44	9.08
300	58.90	48.13	204	2.66	1.03
301	0.0	0.0	401	58.15	67.69
113	0.0	0.0			

An R factor for nuclear plus magnetic intensities of 0.05 was obtained for the $\text{Ho}_2\text{Fe}_{17}$ structure. In all these compounds the value, at low temperature, of the Ho moment was calculated as $9.5 \mu_B \pm 0.2$, just below the value of $10 \mu_B$ calculated for the trivalent free ion, thus providing evidence that the crystal field splitting is low as reported by Moon, et al. [7] for the Laves phase compounds HoCo_2 and ErCo_2 . A temperature study of two magnetic reflections (220 and 222), due only to the Ho moments and to the Fe moments respectively, showed a sharp decrease of the intensity due to the Ho sublattice magnetization while that due to the Fe sublattice remained constant to about

the Curie temperature. From these observations, it was concluded that the Ho-Fe interaction is weak and that the Curie temperature results primarily from the Fe sublattice magnetization, i. e., from the Fe-Fe exchange interactions. The absolute value of the Fe moment was found to fluctuate around a mean value depending upon the crystallographic site but, on the average, the Fe moment increased from $1.7 \mu_B$ in HoFe_2 to $2.1 \mu_B$ in $\text{Ho}_2\text{Fe}_{17}$. This variation is interpreted as an effect of the conduction electrons which fill up the 3 d band, and this effect is more important in HoFe_2 than in $\text{Ho}_2\text{Fe}_{17}$ where there are less electrons provided by the rare earth atoms. The relative non-dependence of the Fe moment on the amount of rare earth present in any of the (R, Fe) systems should be noted. The lowest value of the Fe moment has been found to be $1.45 \mu_B$ in YFe_2 , Givord et al. [8]. However, in the (R, Co) series the moment on Co has been found to depend directly on both the rare earth moment and its concentration in the alloy. No moment has been detected for Co in YCo_2 , Lemaire et al. [9].

Finally, the magnetic behavior of the rare earth-iron alloys is very similar to that of transition metals and alloys where the direct exchange interaction plays a major role in the determination of the magnetic properties.

Slater and Néel [10] have studied and interpreted the variation of the interaction energy on 3 d elements as a function of the distance between the magnetic shells. It was concluded that antiferromagnetism is directly associated with shorter distances between first neighbors and ferromagnetism to longer distances. In the case of the (Ho-Fe) series the lowest Curie temperature (325°K for $\text{Ho}_2\text{Fe}_{17}$) corresponds to the smallest distance between the Fe atoms and thus it is reasonable to interpret the variation of the Curie temperature in these compounds on the basis of the Néel-Slater theory.

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