An Updated Evaluation of the Fe-Gd (Iron-Gadolinium) System

W. Zhang, C. Li, X. Su, and K. Han

Equilibrium Diagram

Figure 1 shows the assessed equilibrium diagram that is taken mainly on the calculated diagram based on thermodynamic modeling by [95Liu], but includes consideration of the experimental work of [69Sav] and the evaluated diagram of [82Kub]. The equilibrium phases include: (1) the liquid, L; (2) four peritectic intermetallic compounds, that is, $Fe_{17}Gd_2$, $Fe_{23}Gd_6$, Fe_3Gd, and Fe_2Gd; and (3) five terminal solid solutions: (αFe), (γFe), (δFe), (αGd), and (βGd). Table 1 presents the three-phase equilibria and pure metal transformation data. In this

evaluation, more comprehensive literature sources were collected. In particular, some pertinent thermodynamic data were found. The liquidus composition at the peritectic equilibrium with Fe_2Gd is ~20 at.% more Gd-rich than the diagram in [Massalski2]. This result is consistent with the review of [96Oka].

The binary phase diagram of the Fe-Gd system has been investigated by several investigators [60Vic, 61Nov, 61Sav, 62Cop, 64Bur, 69Sav]. [82Kub] proposed an Fe-Gd phase diagram based on [62Cop] with some modifications. Recently, [93Oka] evaluated this system. [61Nov] suggested that seven intermet-

**Table 1   Special Points of the Assessed Fe-Gd Phase Diagram**

Reaction	Composition, at.% Fe			Temperature, °C	Reaction type	Reference
L ↔ δFe		100		1538	Melting	[Massalski2]
δFe ↔ γFe		100		1394	Allotropic	[Massalski2]
γFe ↔ αFe		100		912	Allotropic	[Massalski2]
δFe ↔ L + γFe	~99.4	91	~99.45	1380	Metatectic	[69Sav, 95Liu]
γFe + Fe$_{17}$Gd$_2$ ↔ αFe	~99.97	89.5	~99.87	~924	Peritectoid	[69Sav, 82Kub, 95Liu]
βFe$_{17}$Gd$_2$ ↔ αFe$_{17}$Gd$_2$		89.5		1215	Polymorphic	[90Ati2]
L + γFe ↔ Fe$_{17}$Gd$_2$	88.1	~99.1	89.5	1331	Peritectic	[82Kub, 95Liu]
L + Fe$_{17}$Gd$_2$ ↔ Fe$_{23}$Gd$_6$	76.6	89.5	79.3	1283	Peritectic	[69Sav, 82Kub, 95Liu]
L + Fe$_{23}$Gd$_6$ ↔ Fe$_3$Gd	52.3	79.3	75	1156	Peritectic	[95Liu]
L + Fe$_3$Gd ↔ Fe$_2$Gd............................	44	75	66.7	1082	Peritectic	[69Sav, 82Kub]
L ↔ Fe$_2$Gd + αGd................................	~26.4	66.7	~0	~832	Eutectic	[69Sav, 95Liu]
L ↔ βGd		0		1313	Melting	[Massalski2]
βGd ↔ αGd		0		1235	Allotropic	[Massalski2]

Table 2   Crystal Structure Data

Phase	Composition, at.% Fe	Pearson symbol	Space group	Strukturbericht designation	Prototype	Reference
(αGd).........................	0	hP2	P6$_3$/mmc	A3	Mg	[61Nov, 71Bru]
(βGd)..........................	0	cI2	Im$\bar{3}$m	A2	W	[71Bru]
Fe$_2$Gd.........................	66.7	cF24	Fd$\bar{3}$m	C15	Cu$_2$Mg	[64Man, 78Cre]
Fe$_3$Gd.........................	75	hR12	R$\bar{3}$m	...	Be$_3$Nb	[65Smi, 85Sei]
Fe$_{23}$Gd$_6$......................	79.3	cF116	Fm$\bar{3}$m	D8$_a$	Mn$_{23}$Th$_6$	[65Kri]
αFe$_{17}$Gd$_2$....................	89.5	hR19	R$\bar{3}$m	...	Zn$_{17}$Th$_2$	[63Kri, 70Giv]
βFe$_{17}$Gd$_2$....................	89.5	hP38	P6$_3$/mmc	...	Ni$_{17}$Th$_2$	[63Kri, 70Giv]
(αFe)..........................	100	cI2	Im$\bar{3}$m	A2	W	[Massalski2]
(γFe)..........................	100	cF4	Fm$\bar{3}$m	A1	Cu	[Massalski2]
(δFe)	100	cI2	Im$\bar{3}$m	A2	W	[Massalski2]
Questionable phases						
Fe$_3$Gd$_2$	60	...	c*30	...	...	[61Nov]
Fe$_7$Gd$_2$	77.8	...	o*18	...	...	[61Nov]
Fe$_4$Gd.........................	80	hP10	...	...	...	[61Nov]
Fe$_5$Gd.........................	83.3	hP6	P6/mmm	D2$_d$	CaCu$_5$	[60Nas, 61Nov]
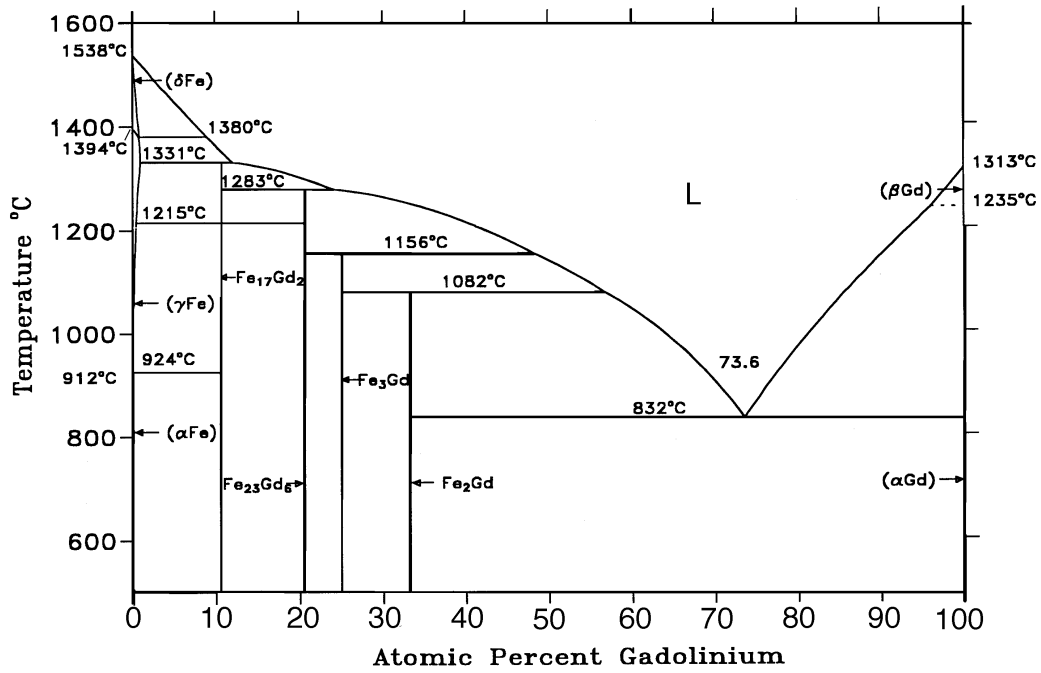
Fig. 1(a) Assessed Fe-Gd phase diagram plotted with composition in at.% Gd. Note the two-phase regions between the (Fe) allotropes are not resolvable on the scale of this diagram.
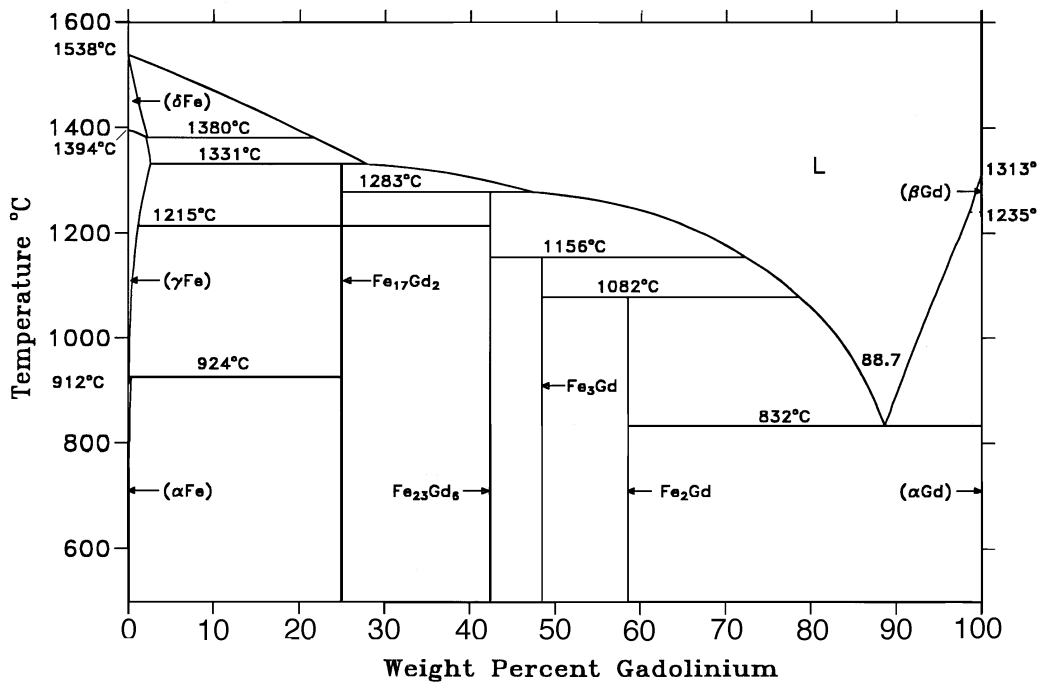
Fig. 1(b) Assessed Fe-Gd phase diagram plotted with composition in wt.% Gd. Note the two-phase regions between the (Fe) allotropes are not resolvable on the scale of this diagram.

allic compounds (Fe$_3$Gd$_2$, Fe$_2$Gd, Fe$_3$Gd, Fe$_7$Gd$_2$, Fe$_4$Gd, Fe$_5$Gd, and Fe$_{17}$Gd$_2$) exist, but compounds Fe$_3$Gd$_2$, Fe$_7$Gd$_2$, and Fe$_5$Gd have not been confirmed by other measurements [61Sav, 62Cop, 69Sav]. [61Sav] reported compounds Fe$_{17}$Gd$_2$ and Fe$_2$Gd, and a third compound, hinted at by thermal analysis. [62Cop] confirmed the existence of the compounds Fe$_9$Gd, Fe$_3$Gd, and Fe$_2$Gd. The compound Fe$_9$Gd may be inferred as

Fe$_{17}$Gd$_2$. According to [Shunk], the phase diagram of [64Bur] included four compounds: Fe$_{17}$Gd$_2$, Fe$_4$Gd, FeGd, and FeGd$_2$. The last two compounds are unusual. [64Bur] probably mistook Fe$_3$Gd and Fe$_2$Gd for FeGd and FeGd$_2$, respectively [93Oka], because Fe$_3$Gd and Fe$_2$Gd occur in the phase diagram of [69Sav] (same research group). [69Sav] showed Fe$_{17}$Gd$_2$ and Fe$_2$Gd as certain with Fe$_4$Gd and Fe$_3$Gd as ques-

Table 3   Fe-Gd Lattice Parameter Data

Phase	Composition, at.% Fe	Lattice parameters, nm a	b	c	Reference
αGd	0	0.3635	...	0.5780	[61Nov, 71Bru]
		0.36336	...	0.5781	[Massalski2]
βGd............................	0	0.406	...	...	[71Bru]
Fe$_2$Gd...........................	66.78	0.7450	...	...	[44End]
		0.7400	...	...	[60Nas]
		0.7530	...	...	[61Nov]
		0.7390	...	...	[60Wer, 62Cop, 68Ray, 87Ich]
		0.7389	...	...	[61Bae]
		0.7360	...	...	[61Sav]
		0.7355	...	...	[64Man]
		0.740	...	...	[78Cre]
		0.73909	...	...	[68Man]
		0.7394	...	...	[72Can, 62Hub]
		0.73875	...	...	[74Atz]
		0.7396	...	...	[70Bus]
		0.7403	...	...	[82Kie]
		0.7390	...	...	[87Ich]
Fe$_3$Gd........................	75	0.3205	...	1.303	[61Nov]
		0.5148	...	2.462	[62Cop, 65Smi]
		0.51692	...	2.4737	[66Van]
		0.51654	...	2.4707	[68Dwi]
		0.5166	...	2.471	[68Ray]
		0.5157	...	2.470	[85Sei]
Fe$_{23}$Gd$_6$........................	79.3	1.2134	...	...	[65Kri]
		1.212	...	...	[86Nag]
βFe$_{17}$Gd$_2$................................	89.5	0.839	...	0.853	[61Nov]
		0.850	...	0.835	[63Kri]
		0.8486	...	0.8349	[66Bus]
		0.8496	...	0.8345	[70Giv]
αFe$_{17}$Gd$_2$	89.5	0.8536	...	1.2429	[61Kri, 61Sav]
		0.855	...	1.240	[63Kri]
		0.8517	...	1.2429	[66Bus]
		0.8538	...	1.2431	[68Ray]
		0.8540	...	1.2428	[70Giv]
αFe	100	0.28665	...	...	[Massalski2]
γFe	100	0.36467	...	...	[Massalski2]
δFe	100	0.29315	...	...	[Massalski2]
Questionable phases					
Fe$_3$Gd........................	60	0.825	...	...	[61Nov]
Fe$_7$Gd$_2$........................	77.8	0.571	0.678	0.715	[61Nov]
Fe$_4$Gd........................	80	0.515	...	0.664	[61Nov]
Fe$_5$Gd........................	83.3	0.50	...	0.41	[61Nov]
		0.492	...	0.411	[61Nov]
		0.483	...	0.413	[62Hub]

tionable. In line with the other Fe-RE systems, the earlier reported Fe₄Gd was written as $Fe_{23}Gd_6$ [Moffatt, 82Kub]. The Fe-Gd binary phase diagram was thermodynamically assessed by [95Liu] and is similar to that given by [82Kub] and [93Oka] with four peritectic intermetallic compounds: $Fe_{17}Gd_2$, $Fe_{23}Gd_6$, Fe_3Gd, and Fe_2Gd, and one eutectic reaction.

Terminal Phases

The Gd dissolves less than 0.6 at.% Fe [62Cop]. The transformation temperature for $\alpha \leftrightarrow \beta$ is 1235 °C [Massalski2]. However, the alternative reports were 1260 °C [82Kub], 1261 °C [63Hul], and 1284 °C [71Bru]. The melting point of Gd was suggested to be 1313 °C by [Massalski2], 1312 °C by [71Bru], and 1315 °C by [63Hul]. The data from [Massalski2] are commonly accepted.

[95Liu] reported 1239 °C as the $\beta Gd \leftrightarrow \alpha Gd + L$ reaction temperature according to his thermodynamic assessment using the data of [91Din] for pure elements. Because there is no experimental data to confirm this reaction, it is not adopted in Fig. 1.

The $\delta Fe \leftrightarrow L + \gamma Fe$ invariant reaction is at 1380 °C [69Sav, 82Kub, 95Liu], and the compositions of the phases are from [95Liu].

Fe₂Gd

This compound was obtained independently by [60Wer], [61Nov], and [78Cre]. It is formed by a peritectic reaction at 1080 °C. The liquidus composition at the peritectic melting of Fe_2Gd is ~56 at.% Gd [95Liu] or ~59 at.% Gd [69Sav], which differs by ~20 at.% from that given by [62Cop], [82Kub], and [93Oka]. In view of the systematic trends of the Fe-RE systems, the diagram of [69Sav] and [95Liu] appears to be more reasonable [96Oka]. The value of [95Liu] is adopted in Fig. 1.

The $L \leftrightarrow Fe_2Gd + (\alpha Gd)$ eutectic is reported at 830 °C, 72 at.% Gd [61Sav, 69Sav]; at 845 °C, 66.9 at.% Gd [62Cop]; at 845 °C, 70 at.% Gd [82Kub]; at 849 °C, 72 at.% Gd [64Bur]; or at 832 °C, 73.6 at.% Gd [95Liu].

Fe₃Gd

The existence of the compound Fe_3Gd was first confirmed by [61Nov] and [62Cop] using thermal, x-ray, and metallographic

methods. Fe_3Gd melts peritectically at 1156 °C with the liquidus composition of ~44 at.% Gd [95Liu] or at 1155 °C with the liquidus composition of ~34 at.% Gd [82Kub, 93Oka]; the former value is adopted in Fig. 1.

Fe₂₃Gd₆

The earlier reported Fe₄Gd [59Nes, 61Nov] should probably be written as $Fe_{23}Gd_6$ with $Mn_{23}Th_6$-type structure [65Kri, 77Bus]. [84Her], [86Nag], and [90Ati1] confirmed the existence of $Fe_{23}Gd_6$. It is likely formed peritectically at 1280 °C [82Kub], but only very slowly [84Her]. The formation of the compound is accelerated by using less pure starting materials, with O as one effective impurity. [93Oka] suggested that $Fe_{23}Gd_6$ may be stable only in a restricted temperature range immediately below the melting point at 1280 °C, whereas other investigators found $Fe_{23}Gd_6$ to be a stable phase at room temperature [92Tia] and at 500 °C [95Zhu].

Fe₁₇Gd₂

This compound melts peritectically at 1331°C [67Liu]. $Fe_{17}Gd_2$ is currently accepted as crystallizing in two modifications: a high-temperature phase with the hexagonal $Ni_{17}Th_2$-type structure and a low-temperature phase with rhombohedral $Zn_{17}Th_2$-type structure with the polymorphic transition temperature being 1215 °C [90Ati2]. Neglecting

Table 4   Experimental Enthalpies of Mixing in the Fe-Gd System at 1850 K

Composition, at.% Gd	$-\Delta H_f$, kJ/mol
0	0
10	1.25 ± 0.14
20	3.09 ± 0.34
30	4.93 ± 0.71
40	6.37 ± 0.91
50	7.21 ± 0.83
60	7.36 ± 0.62
70	6.82 ± 0.42
80	5.66 ± 0.29
90	3.64 ± 0.20
100	0

Table 5   Experimental Enthalpies of Formation in the Fe-Gd System

Compound	ΔH_f, kJ/mol	T, K	Method	Temperature of experiment, K	Reference
Fe₂Gd	−11.6	298	solution calorimetry in liquid Al	998	[86Col]
	−3.5	1078	reaction calorimetry	…	[75Deo]
Fe₃Gd	−9.3	298	solution calorimetry in liquid Al	988	[87Col1]
Fe₁₇Gd₂	−2.3	298	solution calorimetry in liquid Al	1092	[87Col1]

Table 6   Measured T_c and β Values Used in the Assessed Fe-Gd System

Phase	Fe₂Gd	Fe₃Gd	Fe₂₃Gd₆	Fe₁₇Gd₂
T_c, K	782	728	468	472
β, μ_B	3.35	1.6	14.8	21.2

Table 7   Thermodynamic Parameters Obtained by [95Liu] (in SI units)

Liquid	$L_{Fe,Gd}^{0,L} = -27\ 625 + 17.869T$
	$L_{Fe,Gd}^{1,L} = 14\ 594 - 8.894T$
bcc	$L_{Fe,Gd}^{0,bcc} = -28\ 758 + 38.096T$
fcc	$L_{Fe,Gd}^{0,fcc} = 30\ 231$
cph	$L_{Fe,Gd}^{0,cph} = 1\ 000\ 000$
$Fe_{17}Gd_2$..	$G_{Fe:Gd}^{0,Fe_{17}Gd_2} - 17G_{Fe}^{0,hbcc} - 2G_{Gd}^{0,hcph} = -218\ 222 + 98.884T$
$Fe_{23}Gd_6$..	$G_{Fe:Gd}^{0,Fe_{23}Gd_6} - 23G_{Fe}^{0,hbcc} - 6G_{Gd}^{0,hcph} = -430\ 075 + 182.333T$
Fe_3Gd..	$G_{Fe:Gd}^{0,Fe_3Gd} - 3G_{Fe}^{0,hbcc} - G_{Gd}^{0,hcph} = -61\ 393 + 26.214T$
Fe_2Gd..	$G_{Fe:Gd}^{0,Fe_2Gd} - 2G_{Fe}^{0,hbcc} - G_{Gd}^{0,hcph} = -46\ 829 + 63.295T - 5.917T \ln T - 353\ 121T^{-1} - 94\ 463\ 542T^{-3}$

Table 8   Curie Temperature Values in the Fe-Gd System

Phase	Composition, at.% Fe	T_c, K	Reference
Fe_2Gd.......................	66.7	782	[64Man]
		788	[74Dar]
		796	[77Bus]
		810	[85Zho]
Fe_3Gd.......................	75.0	729	[77Bus]
$Fe_{23}Gd_6$....................	79.3	659	[77Bus]
$Fe_{17}Gd_2$....................	89.5	476	[77Bus]

ranges of homogeneity is common when calculating phase diagrams because such neglect greatly simplifies the calculating procedure, and the diagram in Fig. 1 is based primarily on the calculated diagram of [95Liu]. There is strong evidence for a range of homogeneity for $Fe_{17}Gd_2$. Indeed, [81Sta] has reported that the $Zn_{17}Th_2$-type structure occurs only for Fe-deficient stoichiometries, $Fe_{17-x}Th_2$. Further, a range of homogeneity for the phase was reported by [66Bus] who found the rhombohedral $Zn_{17}Th_2$-type structure for annealed alloys across a range of compositions. [66Bus] also found that quenched stoichiometric alloys had the $Ni_{17}Th_2$-type structure while quenched alloys through the composition range $Fe_{17}Gd_2$ and Fe_7Gd showed both the rhombohedral $Zn_{17}Th_2$-type structure and the hexagonal $Ni_{17}Th_2$-type structure. Finally, in quenched alloys near a stoichiometry of Fe_7Gd, [66Bus] found weak reflections from Fe_3Gd mixed with reflections from the $Zn_{17}Th_2$-type structure. Later work by [70Giv] showed that alloys near the composition Fe_7Gd could be indexed on hexagonal lattice parameters of $a = 0.4905$ to 0.4931 nm and $c = 0.4173$ to 0.4143 nm, which are characteristic of the closely related $CaCu_5$-type structure. [70Giv] postulated that such a diffraction pattern could be produced by the substitution of one Gd atom by two Fe atoms (2 to 1 is approximately the atom volume ratio of Gd to Fe) on a significant number of Gd crystallographic sites. Thus there is definite evidence for a range of homogeneity, but composition limits for the homogeneity range await determination.

Metastable Phases

Many compounds reported by early authors [61Nov, 61Gsc, 66Bus] were not confirmed by later investigations. There is the possibility that some of those unconfirmed compounds are metastable phases. Further, there is still a question as to what portion of the reports of [66Bus, 70Giv, 77Bus] represents equilibrium and what represents transient kinetic effects or metastability.

Formation of Amorphous Phases

The ability to form amorphous alloys can be estimated by the imaginary eutectic that is obtained from extrapolation of the terminal liquidus lines of each element. In the Fe-Gd system, the formation range of the amorphous phase shifts from the real eutectic composition (about 70 at.% Gd) toward the virtual eutectic composition (about 50 to 60 at.% Gd). The atomic size effect of constituent elements on the metallic glass formation was discussed by introducing the atomic volume mismatch evaluated from the cube of the atomic radius of solvent and solute [85Uen]. Amorphous Fe-Gd alloys, ribbons about 15 μm thick, from 16 to 70 at.% Gd, were prepared with a melt-quenching method in a vacuum [91Tok]. Samples from 16 to 70 at.% Gd were obtained by [91Yan]. The αGd phase appeared in these samples at higher Gd concentrations. In addition, pure Gd, Fe, and $Fe_{1-x}Gd_x$ thin films were thermally evaporated with a thickness of 500 to 700 Å [84Lee1, 84Lee2]. The composition dependence of the as-deposited material showed three different regions: (1) an amorphous alloy and αFe mixture up to 24 at.% Gd, (2) an amorphous alloy phase in the composition range from 24 to 60 at.% Gd, and (3) αGd and an amorphous alloy mixture above 60 at.% Gd.

Thermal Stabilities of Amorphous Films

Amorphous alloys are in a nonequilibrium state and crystallize to lose their amorphous characteristics above a certain temperature. Several relevant investigations have been carried out on the Fe-Gd alloy system. The results of thermomagnetization [91Yan] showed three types of crystallization processes: (1) αFe, $Fe_{23}Gd_6$, and Fe_2Gd at the composition 22 at.% Gd, (2) αFe, Fe_2Gd, and αGd in the region 33.3 to 58 at.% Gd, and (3) Fe_2Gd and αGd at the composition 70 at.% Gd. The XRD study [91Tok] indicated that these amorphous alloys crystallized into two phases, αGd and the Laves phase (Fe_2Gd) with-

out any trace of the αFe phase. In addition, the investigation of the crystallization process for amorphous thin films by means of in situ transmission electron microscopy [84Lee1, 84Lee2] was characterized by the three reaction stages: (1) αFe and αGd were precipitated by primary crystallization, (2) some transient intermetallic compounds were formed, and (3) the equilibrium phases were formed by subsequent decomposition reactions. During the in situ crystallization reaction, the αFe phase appeared in the first or the second but not the final reaction stage.

The onset temperatures of crystallization are different among different investigations because of different heating times and cooling rates. [91Yan] reported that crystallization did not start below the Curie temperature of any amorphous alloy. This result is in accordance with that of x-ray measurement [91Tok] but different from that for bulk ribbon (60 at.% Gd) obtained by [79Bus] who reported that αGd began to precipitate around 140 °C.

Magnetic Properties of Amorphous Alloy Films

The evaporated amorphous film of Fe-Gd was reported to possess a perpendicular anisotropy sufficient to cause the magnetization to be normal to the film plane [74Hei], particularly in the vicinity of the magnetic compensation point* [78Mim]. The mean field model [75Hei, 76Hei] was proposed to calculate a systematic variation of the Curie temperature associated with a variation of composition and rare earth species and also to reproduce the observed shape of magnetization-versus-temperature curves. [78Mim], [84Lee1], and [91Yan] investigated the Curie temperature, T_{ca}, and the compensation temperature, T_{comp}, for amorphous Fe-Gd alloys at different compositions.

Crystal Structures and Lattice Parameters

Crystal structure and lattice parameter data for the phases in the Fe-Gd system are summarized in Tables 2 and 3.

Thermodynamics

The specific heat anomaly of Fe$_2$Gd, a singularity in the heat capacity around the magnetic ordering temperature, was measured and discussed by [74Dar]. The lower temperature specific heat was determined in the temperature range 8 to 300 K [81Ger1]. The crystal field contribution to the heat capacity was evaluated [81Ger2]. The Gd^{3+} is an *s*-state ion and as such is not expected to interact with the crystalline electric field. However, [81Ger2] illustrated that this contribution was significant. The heat capacity of Fe$_2$Gd intermetallic compound over the temperature region 1.5 to 10 K was also measured [79But]. Values for the apparent electronic heat capacity between 5 and 10 K were determined as $C_p = \Gamma'T + T^3\beta$ with coefficients $\Gamma' = 19.3$ mJ/mole-K^2, and $\beta = 0.296$ mJ/mole-K^4.

A molecular field model for analytically predicting entropy change in the temperature region $T \geq T_c$ was developed for the Fe-Gd system at the composition 89.5 at.% Fe [84Oes].

Enthalpies of mixing for liquid alloys were measured at 1850 K by [89Nik] (Table 4). The enthalpies of formation of transition rare earth metal alloys were collected by [87Col2]; these include values for Fe$_2$Gd, Fe$_3$Gd, and Fe$_{17}$Gd$_2$ compounds (Table 5). The phase relations and thermodynamic data of the Fe-Gd system were thermodynamically assessed by [95Liu].

For some phases, there is a magnetic transformation. According to [78Hil], the magnetic contribution to the Gibbs energy, $G_m^{mg,\varphi}$, in the structure φ is described by:

$$G_m^{mg,\varphi} = RT \ln (\beta^\varphi + 1)f(\tau)$$

$$\tau = T/T_c^\varphi \qquad\qquad (Eq\ 1)$$

where T_c^φ is the critical (Curie or Neel) temperature and β^φ the magnetic moment, $f(\tau)$ are the polynomials generated by [78Hil]. T_c and β are taken from the measured critical temperature and the mean Bohr magnetic moment per mole. Table 6 lists the values of T_c and β used by [95Liu].

Thermodynamic Models of Liquid, fcc, bcc, and cph Phases

The liquid, fcc, bcc, and cph phases are treated by a one-sublattice model for which the Gibbs energy expression is:

$$G_m^\varphi = X_{Fe}G_{Fe}^{0,\varphi} + X_{Gd}G_{Gd}^\varphi + RT(X_{Fe} \ln X_{Fe} + X_{Gd} \ln X_{Gd})$$

$$+ G_m^{mg,\varphi} + X_{Fe}X_{Gd} \sum_i L_{Fe,Gd}^{i,\varphi} (X_{Fe} - X_{Gd})^i \qquad (Eq\ 2)$$

where X_i is the mole fraction of element i (i = Fe, Gd), $G_i^{0,\varphi}$ is the molar Gibbs energy in the structure φ in nonmagnetic states, $L_{Fe,Gd}^{i,\varphi}$ are the binary interaction parameters, and $G_m^{mg,\varphi}$ is the magnetic contribution to the Gibbs energy.

Thermodynamic Models of Intermetallic Compounds

All the intermetallic compounds are treated as stoichiometric phases. Their Gibbs energies per mole of formula unit Fe$_A$Gd$_B$ can be expressed as:

$$G_m^{0, Fe_AGd_B} = A\ G_{Fe}^{0, hbcc} + B\ G_{Gd}^{0, hcph} + a + bT + cT \ln T$$

$$+ G_m^{0,mg,Fe_AGd_B} \qquad (Eq\ 3)$$

where $G_{Gd}^{0,hcph}$ and $G_{Fe}^{0,hbcc}$ are the Gibbs energies of the respective pure elements in a hypothetical nonmagnetic cph and bcc structure, and G_m^{0,mg,Fe_AGd_B} is the magnetic contribution to the Gibbs energy.

---

* The ferromagnetic coupling of Fe when in combination with heavy rare earth elements such as Gd causes a decrease in the spontaneous magnetization, M_s, with increasing temperature, whereas the antiferromagnetic coupling of Gd causes an increase in the spontaneous magnetization with increasing temperature. The temperature at which the increase due to Gd matches the decrease due to Fe is known as the compensation temperature.

The thermodynamic data for pure elements are from the work of [91Din] with reference to SER (standard element reference) at 298.15 K.

A consistent thermodynamic description of this system obtained by [95Liu] is given in Table 7. The calculated phase equilibria agree well with the literature data [61Sav, 69Sav].

Magnetism

The magnetic properties of the intermediate phases have been investigated in various laboratories [71Kir, 74Kli, 74Dar, 64Man, 59Nes, 81Ger]. [77Bus] has compiled the magnetic data for various rare earth/transition metal compounds and lists mean values. [85Zho] studied the magnetic properties of Fe_2Gd. The Curie temperatures of the compounds in the Fe-Gd system are given in Table 8.

Cited References

*44End: F. Endter and W. Klemm, Crystal Structures of Fe_2Gd and Mn_2Gd, *Z. Anorg. Chem., 252,* 377-379 (1944) in German. (Crys Structure; Experimental)

59Nes: E.A. Nesbitt, J.H. Wernick, and E. Corenzwit, Magnetic Moments of Alloys and Compounds of Iron and Cobalt with Rare Earth Metal Additions, *J. Appl. Phys., 30*(3), 365-367 (1959). (Magnetism; Experimental)

60Nas: K. Nassau, L.V. Cherry, and W.E. Wallace, Intermetallic Compounds between Lanthanons and Transition Metals of the First Long Period, *Phys. Chem. Solids, 16,* 123-130 (1960). (Crys Structure; Experimental)

60Vic: R.C. Vickery, W.C. Sexton, V.F. Novy, and E.V. Kleber, Magneto Structural Studies on Gadolinium-Iron Alloys, *J. Appl. Phys., 31*(5), Supplement 366S-367S (1960). (Equi Diagram; Experimental)

60Wer: J.H. Wernick and S. Geller, Rare-Earth Compounds with the $MgCu_2$ Structure, *Trans. Met. Soc. AIME, 218*(10), 866-868 (1960). (Equi Diagram; Experimental)

61Bae: N.C. Baenziger and J.L. Moriarty, Gadolinium and Dysprosium Intermetallic Phases, *Acta Crystallogr., 14,* 948-950 (1961). (Crys Structure; Experimental)

61Gsc: K.A. Gschneidner, *Binary Alloy Systems, Rare Earth Alloys,* Vol. 186, van Nostrand, New York (1961). (Meta Phases; Review)

*61Kri: P.I. Kripyakevich and E.I. Gladyshevski, Crystal Structure of Compounds in the Nd-Al, Y-Al, and Gd-Fe Systems, *Kristallografiya, 6*(1), 118 (1961) in Russian; TR: *Sov. Phys. Crystallogr., 6*(1), 95 (1961). (Crys Structure; Experimental)

61Nov: V.F. Novy, R.C. Vickery, and E.V. Kleber, The Gadolinium-Iron System, *Trans. Met. Soc. AIME, 221,* 580-585 (1961). (Equi Diagram, Meta Phases, Crys Structure; Experimental; #)

61Sav: E.M. Savitskii, V.F. Terekhova, I.V. Burov, and O.D. Chistyakov, Equilibrium Diagram for Alloys of the Gadolinium-Iron System, *Russ. J. Inorganic Chem., 6*(7), 883-885 (1961). (Equi Diagram, Crys Structure, Thermo; Experimental; #)

62Cop: M.I. Copeland, M. Krug, C.E. Armantrout, and H. Kato, "Iron-Gadolinium Phase Diagram," Report of Investigations, No. 5925, U.S. Bureau of Mines (1962). (Equi Diagram, Crys Structure; Experimental)

62Hub: W.M. Hubbard and E. Adams, Intermetallic Compounds of Iron and Cobalt with Gadolinium, *J. Phys. Soc. Jpn., 17* (suppl. B-I), 143-146 (1962). (Crys Structure; Experimental)

63Hul: R.D. Hultgren, R.L. Orr, P.D. Anderson, and K.K. Kelly, *Selected Values of Thermodynamic Properties of Metals and Alloys,* Wiley, New York (1963). (Equi Diagram; Experimental)

*63Kri: P.I. Kripyakevich, V.F. Terekhova, O.S. Zarechnyuk, and I.V. Burov, Crystal Structures of Some Intermetallic Compounds of Gadolinium and Neodymium, *Kristallografiya, 8*(2), 203 (1963); TR: *Sov. Phys. Crystallogr.* (Crys Structure; Experimental)

*64Bur: I.V. Burov, V.F. Terekhova, and E.M. Savitskii, *Voprosy Teoriii Primeneiya Redkozemelnykh Metallov,* E.M. Savitskii and V.F. Terekhova, Ed., Akademiya Nauk SSSR, Moscow, 116-123 (1964); quoted in [Shunk]. (Equi Diagram; Experimental; #)

64Man: M. Mansmann and W.E. Wallace, Magnetic Properties of $GdFe_2$ and $DyFe_2$, *J. Chem. Phys., 40,* 1167-1168 (1964). (Crys Structure, Magnetism; Experimental)

*65Kri: P.I. Kripyakevich, D.P. Frankevich, and Y.V. Voroshilov, Compounds with Structures of the Th_6Mn_{23} Type in Alloys of Rare Earth Metals with Manganese and Iron, *So. Porosh. Met., 11,* 55-61 (1965). (Equi Diagram, Crys Structure; Experimental)

65Smi: J.F. Smith and D.A. Hansen, The Structures of YNi_3, YCo_3 $ThFe_3$ and $GdFe_3$, *Acta Crystallogr., 19,* 1019-1024 (1965). (Crys Structure; Experimental)

66Bus: K.H.J. Buschow, The Crystal Structures of the Rare-Earth Compounds of the Form R_2Ni_{17}, R_2Co_{17} and R_2Fe_{17}, *J. Less-Common Met., 11,* 204-208 (1966). (Meta Phases, Crys Structure; Experimental)

66Van: J.H.N. Van Vucht, Note on the Structures of $GdFe_3$, $GdNi_3$, $GdCo_3$ and the Corresponding Yttrium Compounds, *J. Less-Common Met., 10,* 146-147 (1966). (Crys Structure; Experimental)

68Dwi: A.E. Dwight, "The Unit-Cell Constants of Some $PuNi_3$-Type Compounds," *Acta Crystallogr. B, 24,* 1395-1396 (1968). (Crys Structure; Experimental)

68Man: R.C. Mansey, G.V. Raynor, and I.R. Harris, Rare-Earth Intermediate Phases, V. The Cubic Laves Phases Formed by Rare-Earth Metals with Iron and Nickel, *J. Less-Common Met., 14,* 329-336 (1968). (Crys Structure; Experimental)

68Ray: A.E. Ray, Iron-Rare Earth Intermediate Phase, *Proc. 7th Rare Earth Research Conference,* Gordon and Breach, Coronado, CA, 473-484 (1968). (Crys Structure; Experimental)

69Sav: E.M. Savistkii, V.F. Terekhova, R.S. Torchinova, I.A. Markova, O.P. Naumkin, V.E. Kolesnichenko, and V.F. Stroganova, *Proc. Conf. Les Elements des Terres Rares, 1*(180), Paris-Grenole, 49-60 (5-10 May 1969). (Equi Diagram, Thermo; Experimental)

70Bus: K.H.J. Buschow and R.P. van Stapele, Magnetic Properties of Some Cubic Rare-Earth-Iron Compounds of the Type RFe_2 and $R_xY_{1-x}Fe_2$, *J. Appl. Phys., 4*(10), 4066-4069 (1970). (Crys Structure; Experimental)

70Giv: F. Givord and R. Lemaire, Crystalline Structures of the Intermetallic Compound $(Gd_{2/3}Fe_{1/3})Fe_5$, *J. Less-Common Met., 21,* 463-468 (1970) in French. (Equi Diagram, Meta Phases, Crys Structure; Experimental)

*71Bru: G. Bruzzone, M.L. Fornasini, and F. Merlo, The Gadolinium-Cadmium System, *J. Less-Common Met., 25,* 295-301 (1971). (Equi Diagram, Crys Structure; Experimental)

71Kir: H.R. Kirchmayr and W. Steiner, Magnetic Order of the Compound Series $RE_6(Mn_xFe_{1-x})_{23}$, (RE = Y, Gd), *J. Phys., C1,* 665-667 (1971). (Magnetism; Experimental)

72Can: J.F. Cannon, D.L. Robertson, and H.T. Hall, Synthesis of Lanthanide-Iron Laves Phases at High Pressure and Temperatures, *Mater. Res. Bull., 7,* 5-12 (1972). (Crys Structure; Experimental)

74Atz: U. Atzmony and M.P. Dariel, Magnetic Anisotropy and Hyperfine Interactions in $CeFe_2$, $GdFe_2$ and $LuFe_2$, *Phys. Rev. B, 10,* 2060-2067 (1974). (Crys Structure; Experimental)

74Dar: M.P. Dariel, U. Atzmony, and R. Guiser, Specific Heat Anomalies at the Magnetic Ordering Temperatures of Rare Earth-Iron Laves Compounds, *J. Less-Common Met., 34,* 315-319 (1974). (Thermo, Magnetism; Experimental)

74Hei: N. Heiman, A. Onton, D.F. Kyser, K. Lee, and C.R. Guarnieri, Uniaxial Anisotropy in Rare Earth (Gd,Ho,Tb)-Transition Metal (Fe,Co) Amorphous Films, *AIP Conf. Proc., 24,* 573 (1974). (Meta Phases; Experimental)

74Kli: H. Klimker, M. Rosen, M.P. Dariel, and U. Atzmony, Elastic and Magnetoelastic Properties of Polycrystalline Rare-Earth-Iron Laves Compounds, *Phys. Rev. B, 10*(7), 1968-2973 (1974). (Magnetism; Experimental)

75Deo: S.S. Deodhar and P.J. Ficalora, A Study of the Reaction Kinetics for the Formation of Rare Earth-Transition Metal Laves Compounds, *Metall. Trans. A, 6A,* 1909-1914 (1975). (Thermo; Experimental)

75Hei: N. Heiman, K. Lee, and R.I. Potter, Exchange Coupling in Amorphous Rare Earth-Iron Alloys, *AIP Conf. Proc., 29,* 130 (1975). (Meta Phases; Theory)

76Hei: N. Heiman, K. Lee, R.I. Potter, and S. Kirkpatrick, Modified Mean-Field Model for Rare-Earth-Iron Amorphous Alloys, *J. Appl. Phys., 47,* 2634 (1976). (Meta Phases; Theory)

77Bus: K.H.J. Buschow, Intermetallic Compounds of Rare-Earth and $3d$ Transition Metals, *Rep. Prog. Phys., 40,* 1179-1256 (1977). (Equi Diagram, Meta Phases, Magnetism; Review)

78Cre: D.C. Creagh and S.H. Ayling, X-Ray Diffraction Studies of $GdFe_2$ Mössbauer Samples, *J. Mater. Sci., 13,* 113-118 (1978). (Equi Diagram, Crys Structure; Experimental)

78Hil: M. Hillert and M. Jarl, A Model for Alloying Effects in Ferromagnetic Metals, *Calphad, 2*(3), 227-238 (1978). (Thermo; Theory)

78Mim: Y. Mimura, N. Imamura, T. Kobayashi, A. Okada, and Y. Kushiro, Magnetic Properties of Amorphous Alloy Films of Fe with Gd, Tb, Dy, Ho, or Er, *J. Appl. Phys., 49,* 1208 (1978). (Meta Phases; Experimental)

79Bus: K.H.J. Buschow, Crystallization and Magnetic Properties of Amorphous Gd-Fe and Er-Fe Alloys, *J. Less-Common Met., 66,* 89 (1970). (Meta Phases; Experimental)

79But: R.A. Butera, T.J. Clinton, A.G. Moldovan, et al., Heat Capacity Studies of RFe_2 Intermetallic Compounds over the Temperature Region 1.5-10 K (R = Gd, Tb, Dy, Ho, Er, Tm and Lu), *J. Appl. Phys., 50*(11), 7492-7494 (1979). (Thermo; Experimental)

81Ger1: D.J. Germano and R.A. Butera, Heat Capacity and Thermodynamic Functions of the RFe_2 Compounds (R = Gd, Tb, Dy, Ho, Er, Tm, Lu) over the Temperature Region 8-300 K, *J. Solid-State Chem., 37,* 383-389 (1981). (Thermo; Experimental)

81Ger2: D.J. Germano and R.A. Butera, Heat Capacity of, and Crystal-field Effects in, the RFe_2 Intermetallic Compounds, *Phys. Rev. B, 24*(7), 3912-3927 (1981). (Thermo; Experimental)

81Sta: H.H. Stadelmaier and H.K. Park, The System Iron-Gadolinium-Carbon and Its Ternary Carbides, *Z. Metallkde., 72,* 417-422 (1981). (Equi Diagram; Experimental)

82Kie: H.A. Kiers, The Hydrides of YFe_2 and $GdFe_2$, *J. Less-Common Met., 86,* L1-L4 (1982). (Crys Structure; Experimental)

82Kub: O. Kubaschewski, *Iron-Gadolinium, Iron-Binary Phase Diagrams,* Springer-Verlag, New York, 106-107 (1982). (Equi Diagram; Review; #)

84Her: J.F. Herbst and J.J. Croat, Magnetization of R_6Fe_{23} Intermetallic Compounds: Molecular Field Theory Analysis, *J. Appl. Phys., 55*(8), 3023-3027 (1984). (Equi Diagram; Experimental)

84Lee1: S.R. Lee and A.E. Miller, Crystallization and Ferromagnetic Resonance Behavior of Evaporated Gd-Fe Alloy Films, *J. Appl. Phys., 55,* 1745 (1984). (Meta Phases; Experimental)

84Lee2: S.R. Lee and A.E. Miller, Crystallization and Behavior of Evaporated Gd-Fe Alloy Films, *J. Appl. Phys., 55,* 3465 (1984). (Meta Phases; Experimental)

84Oes: H. Oesterreicher and F.T. Park, Magnetic Cooling Near Curie Temperature above 300 K, *J. Appl. Phys., 55*(12), 4334-4338 (1984). (Thermo; Experimental)

85Sei: D. Seitabla, The Study of the Magnetic Behaviors of Some Compounds between Gadolinium and Transition Metals, *Stud. Cercet. Fiz. 37*(1), 27-75 (1985). (Crys Structure; Experimental)

85Uen: S. Ueno and Y. Waseda, Atomic Size Effect on the Glass Formability of Metallic Alloys, *Sci. Rep. Res. Inst. Tôhoku Univ. A, 32*(2), 97-110 (1985). (Meta Phases; Theory)

85Zho: W.D. Zhong, Magnetism of Pseudobinary Rare Earth-Iron Compounds in Cubic Laves Phases, *Res. Met. Mater., 11*(6), 1-12 (1985) in Chinese. (Magnetism; Review)

86Col: C. Colinet and A. Pasturel, Electronic Structure and Enthalpies of Formation of $Gd(Ni,Co,Fe)_2$ Compounds, *J. Less-Common Met., 119,* 167-174 (1986). (Thermo; Experimental)

86Nag: H. Nagai, N. Oyama, Y. Ikami, H. Yoshiem, and A. Tsujimura, The Magnetic Properties of Pseudo-Binary Compounds, $Gd(Fe_{1-x}Mn_x)_2$ and $Gd_6(Fe_{1-y}Mn_y)_{23}$, *J. Phys. Soc. Jpn., 55*(1), 177-183 (1986). (Equi Diagram, Crys Structure; Experimental)

87Col1: C. Colinet, A. Pasturel, and K.H.J. Buschow, Study of the Enthalpies of Formation in the Gd-(Fe, Co, Pd, Pt) Systems, *Metall. Trans. A, 18A,* 903-907 (1987). (Thermo; Experimental)

87Col2: C. Colinet and A. Pasturel, A Data Base for Enthalpies of Formation of Transition Rare-Earth Metal Alloys, *Calphad, 11*(4), 323-334 (1987). (Thermo; Review)

87Ich: K. Ichinose, NMR Study of $Gd(T_{1-x}Co_x)2$ (T = Mn, Fe, Ni, Al), *J. Phys. Soc. Jpn., 56*(8), 2908-2917 (1987). (Crys Structure; Experimental)

89Nik: I.V. Nikolaenko, "Enthalpy of Mixing and Nature of the Interaction of the Components in Gadolinium Melts with 3d-Transition Metals," *Ivz. Akad. Nauk SSSR Met., 4,* 191-194 (1990). (Thermo; Experimental)

90Ati1: S. Atiq, R.D. Rawlings, and D.R.F. West, Phase Relations in the Fe-Co-Gd System, *J. Mater. Sci. Lett., 9,* 518-519 (1990). (Equi Diagram; Experimental)

*90Ati2: S. Atiq, R.D. Rawlings, and D.R.F. West, Crystal Structure of Compounds $Fe_{17}Gd_2$ and $Fe_{17}Tb_2$, *Mater. Sci. Technol., 6*(8), 778-780 (1990). (Crys Structure; Experimental)

91Din: A. Dinsdale, SGTE Data for Pure Element, *Calphad, 15*(4), 317-425 (1991). (Equi Diagram, Thermo; Review)

91Tok: K. Tokumitsu, Crystallization Process and Mössbauer Study of the Melt-Quenched Amorphous Fe-Gd Alloys, *J. Less-Common Met., 170,* 45 (1991). (Meta Phases; Experimental)

91Yan: K. Yano, K. Tokumitsu, E. Kita, H. Ino, and A. Tasaki, Crystallization Behavior and Curie Temperature for Melt-Spun Amorphous $Fe_{100-x}Gd_x(18 \le x \le 70)$ Alloys, *Jpn. J. Appl. Phys., 30*(3B), L482 (1991). (Meta Phases; Experimental)

92Tia: J.H. Tian, J.K. Liang, S.S. Xie, C. Chen, and Y.Q. Wang, The Gd-Fe-Ti Ternary System Section at Room Temperature and the Crystal Structure, *Sci. China Ser. A (CHN), 35*(5), 505-511 (1992). (Equi Diagram; Experimental)

93Oka: H. Okamoto, *Phase Diagrams of Binary Iron Alloys,* H. Okamoto, Ed., ASM International, Materials Park, OH, 152-155 (1993). (Equi Diagram; Review)

95Liu: Z.K. Liu, W. Zhang, and B. Sundman, Thermodynamic Assessment of the Co-Fe-Gd Systems, *J. Alloy. Compd., 226,* 33-45 (1995). (Equi Diagram, Thermo; Theory)

95Zhu: Y.H. Zhuang, J.L. Huang, and H.Y. Zhou, Phase Relations in the Ternary System Gd-Nb-Fe at 500 °C, *Z. Metallkde., 86,* 253-255 (1995). (Equi Diagram; Experimental)

96Oka: H. Okamoto, Fe-Gd (Iron-Gadolinium), *J. Phase Equilibria, 17*(6), 552 (1996). (Equi Diagram; Review)

*Indicates key paper.
#Indicates presence of a phase diagram.