

Experimental Determination and Thermodynamic Calculation of Phase Equilibria in the Fe-Mn-Al System

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The phase equilibria among the face-centered cubic (fcc), body-centered cubic (bcc), and β Mn phases at 800, 900, 1000, 1100, and 1200 °C were examined by electron probe microanalysis (EPMA), and the A2/B2 and B2/D0₃ ordering temperatures were also determined using the diffusion couple method and differential scanning calorimetry (DSC). The critical temperatures for the A2/B2 and B2/D0₃ ordering were found to increase with increasing Mn content. Thermodynamic assessment of the Fe-Mn-Al system was also undertaken with use of experimental data for the phase equilibria and order-disorder transition temperatures using the CALPHAD (Calculation of Phase Diagrams) method. The Gibbs energies of the liquid, α Mn, β Mn, fcc, and ϵ phases were described by the subregular solution model and that of the bcc phase was represented by the two-sublattice model. The thermodynamic parameters for describing the phase equilibria and the ordering of the bcc phase were optimized with good agreement between the calculated and experimental results.

Keywords CALPHAD, magnetic ordering, order-disorder transition, phase diagram, thermodynamic database

1. Introduction

Fe-Mn-Al alloys are the basic system for austenitic stainless steels without Ni and Cr, cryogenic alloys, heat-resistant steels, and magnetic materials [1978Ban, 1981Cha, 1984Den]. In addition, Fe-Al alloys have recently attracted interest as low-density alloys due to cost considerations. Widening the face-centered cubic (fcc) phase region by the addition of Mn to Fe-Al alloys is very useful for improving their toughness because Fe-Al binary alloys with the ordered body-centered cubic (bcc) phase are brittle. The phase equilibria in this system have been studied by various researchers [1933Kos, 1959Sch, 1977Cha, 1989Sat] and Ran has made a critical review of the phase equilibria in the Fe-Mn-Al ternary system [1992Ran]. Recently, Liu et al. [1993Liu1, 1993Liu2, 1996Liu1] carried out detailed investigations including experiments and thermodynamic calculation. However, the thermodynamic parameters evaluated by their calculation [1993Liu2] are based on the magnetic model of Nishizawa et al. [1983Nis], which is different from the Hillert and Jarl model [1978Hil] widely used in

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Thermo-Calc software, and the lattice stabilities of pure elements are also slightly different from those reported by Dinsdale [1991Din]. On the other hand, Liu et al. [1996Liu2] have reinvestigated the phase diagram in the Mn-Al binary system and found that the hexagonal close-packed (hcp) phase region is wider than that indicated by the previous data and that A2/B2 ordering exists in this system. Therefore, additional data for the phase equilibria in the Fe-Mn-Al ternary system are required for reinvestigation; this includes both experiments and thermodynamic calculation. The three sub-binary systems constituting the Fe-Mn-Al ternary system are shown in Fig. 1.

The purpose of the current study was to determine the phase equilibria and the order-disorder transition tempera-

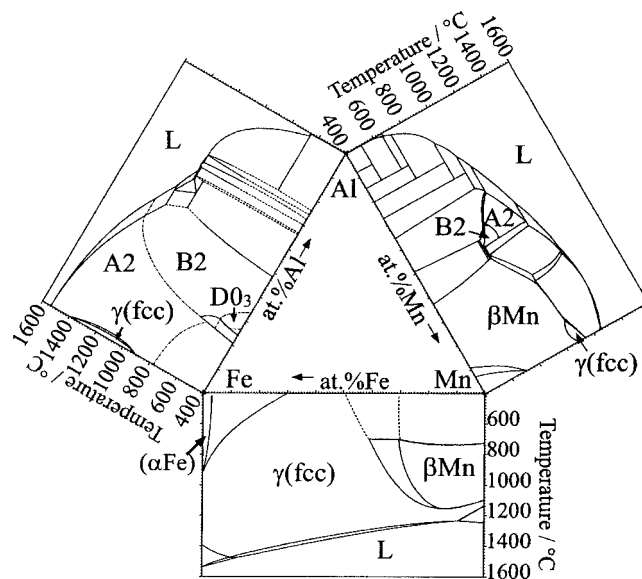


Fig. 1 Binary phase diagrams constituting the Fe-Mn-Al ternary system

tures in the Fe-Mn-Al system and to carry out thermodynamic calculation of the Fe-Mn-Al system including the order-disorder transition.

2. Experimental Procedure

Ternary Fe-Mn-Al alloys were prepared in alumina crucibles by melting electrolytic Fe (99.9%), electrolytic Mn (99.9%), and Al (99.7%) in a high frequency induction furnace under an argon atmosphere. All samples were sealed in quartz capsules under vacuum and treated at 1200 °C for 1 h for homogenization. The specimens were annealed in the range from 800-1200 °C for 336-14 h, and then quenched into water. The microstructures of specimens were examined by optical microscopy. The equilibrium compositions of fcc, bcc, and βMn phases were measured by electron probe microanalysis (EPMA) and were determined by more than five calibrated data by the ZAF (Z: atomic number effect, A: absorption effect, F: fluorescence effect) correction for each phase.

The A2/B2 and B2/D0₃ order-disorder transition temperatures ($T_C^{A2/B2}$ and $T_C^{B2/D03}$) were determined by the diffusion couple method and differential scanning calorimetry (DSC). Details of the preparation of diffusion couples and the determination of the phase equilibria were described in the previous papers [1984Hao, 1998Liu]. The diffusion couples were sealed in transparent quartz capsules and equilibrated in the temperature range from 800 to 1100 °C for 336-24 h, and quenched in water. Following optical metallographic examination of the quenched diffusion couples, the concentration-penetration curve for each element was determined by EPMA along the diffusion-flux direction in each diffusion couple. The compositions associated with the sharp change of curvature in the concentration profile correspond to the critical compositions of ordering [1984Hao, 1998Ish, 2000Kai]. This change in curvature arises from the difference in interdiffusivity of the atoms between the ordered and the disordered phases.

DSC experiment was also used to determine the critical temperature of ordering transitions. DSC measurements were conducted at heating and cooling rates of 5 °C/min or less on specimens kept in a flowing argon atmosphere with Al₂O₃ as a reference.

3. Thermodynamic Models

3.1 Solution Phases

Gibbs energies of the liquid, αMn, βMn, fcc, and ε phases were formulated using the substitutional solution model. According to this model, the integral molar Gibbs energy of a phase φ in a ternary system is given by:

$$G_m^\phi = \sum_{i=Al,Fe,Mn} x_i^\phi \circ G_i^\phi + RT \sum_{i=Al,Fe,Mn} x_i^\phi \ln x_i^\phi + {}^{ex}G_m^\phi \quad (\text{Eq 1})$$

where $\circ G_i^\phi$ is the Gibbs energy of the pure element i in the structural state φ, and ${}^{ex}G_m^\phi$ is the excess molar Gibbs en-

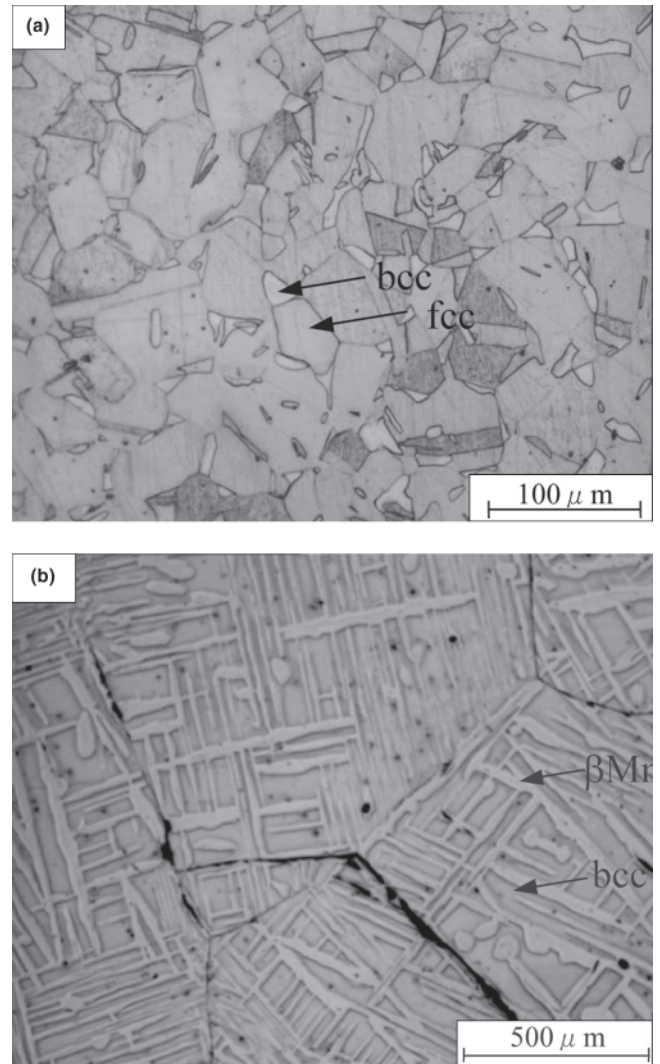


Fig. 2 Microstructures of (a) Fe-20Mn-10Al alloy annealed at 800 °C for 336 h and (b) Fe-30Mn-30Al annealed at 900 °C for 98 h (compositions in at.%)

ergy. The excess Gibbs energy of the ternary system can be written in the Redlich-Kister format [1948Red]:

$$\begin{aligned} {}^{ex}G_m^\phi &= x_{Al}^\phi x_{Fe}^\phi L_{Al,Fe}^\phi + x_{Al}^\phi x_{Mn}^\phi L_{Al,Mn}^\phi + x_{Fe}^\phi x_{Mn}^\phi L_{Fe,Mn}^\phi \\ &\quad + x_{Al}^\phi x_{Fe}^\phi x_{Mn}^\phi L_{Al,Fe,Mn}^\phi \\ L_{i,j}^\phi &= \sum_{m=0}^n {}^mL_{i,j}^\phi (x_i - x_j)^m \\ L_{Al,Fe,Mn}^\phi &= x_{Al}^0 L_{Al,Fe,Mn}^\phi + x_{Fe}^1 L_{Al,Fe,Mn}^\phi + x_{Mn}^2 L_{Al,Fe,Mn}^\phi \end{aligned} \quad (\text{Eq 2})$$

where $L_{i,j}^\phi$ and $L_{Al,Fe,Mn}^\phi$ correspond to the interaction parameters in the binary and ternary systems, respectively. ${}^mL_{i,j}^\phi$ and ${}^nL_{Al,Fe,Mn}^\phi$ are temperature-dependent parameters, which are estimated on the basis of the available thermodynamic and phase diagram data.

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Table 1 Equilibrium compositions of the Fe-Mn-Al system determined in the present work

Temperature, °C	Equilibrium compositions, at. %								
	bcc		fcc		βMn				
	Mn	Al	Mn	Al	Mn	Al			
800	15.0	12.6	21.1	8.7			
	16.4	13.4	22.3	9.6			
	24.4	16.0	29.8	12.3			
	25.5	16.6	31.4	12.7			
	25.8	16.8	32.5	13.1	36.7	16.5			
	40.4	10.3	42.1	14.0			
	38.8	12.6	40.7	14.6			
	38.8	14.1	39.2	15.4			
	61.5	1.0	64.0	1.1			
	44.7	7.0	50.8	9.3			
	23.4	24.0	32.3	23.7			
	23.6	24.1	32.2	23.9			
	23.6	23.8	32.5	23.3			
	22.9	27.8	32.7	25.5			
	23.9	30.8	34.2	27.4			
	26.7	34.5	37.7	29.8			
	30.4	38.2	42.0	32.5			
	900	15.5	12.1	19.9	8.8		
		17.0	12.8	21.3	9.7		
		24.8	15.4	29.1	12.1		
26.3		15.7	30.5	12.5			
27.7		16.1	31.6	13.1			
31.2		16.9	34.8	13.6	39.1	16.5			
...		...	36.7	13.1	40.3	15.8			
...		...	41.4	12.4	43.3	14.6			
...		...	50.5	9.2	52.1	10.2			
30.6		20.9	37.4	21.0			
28.3		26.1	35.1	25.6			
27.7		29.1	35.1	27.2			
30.2		33.7	38.3	30.2			
1000	16.5	11.5	19.8	9.0			
	18.0	12.1	21.2	9.6			
	26.0	14.8	29.3	11.9			
	27.9	14.6	30.9	11.9			
	35.8	15.9	38.6	13.5			
	37.0	16.2	39.7	13.7			
	39.7	16.2	42.4	13.6			
1100	18.9	11.2	21.2	9.1			
	17.7	10.9	20.1	8.7			
	27.0	13.2	29.1	10.7			
	37.4	14.5	39.3	12.3			
	36.1	14.4	38.3	12.2			
...	...	58.4	13.1	57.4	14.7				
1200	19.2	9.8	20.5	8.0			
	28.6	10.8	30.3	9.2			
	39.6	11.9	41.0	10.2			

3.2 bcc Phase

To describe the ordering in the bcc phase, the Gibbs energy of the bcc phase was described on the basis of a two-sublattice split compound energy formalism (s-CEF) [1997Ans, 1998Ohn]:

$$G_m^\phi = G_m^\phi(x_i) + \Delta G_m^{\text{ord}}(y_i^{(s)}) \quad (\text{Eq 3})$$

where $G_m^\phi(x_i)$ is the Gibbs energy of the disordered solution ϕ of the primitive structure corresponding to the ordered phase Φ . $\Delta G_m^{\text{ord}}(y_i^{(s)})$ is the ordering energy extracted from

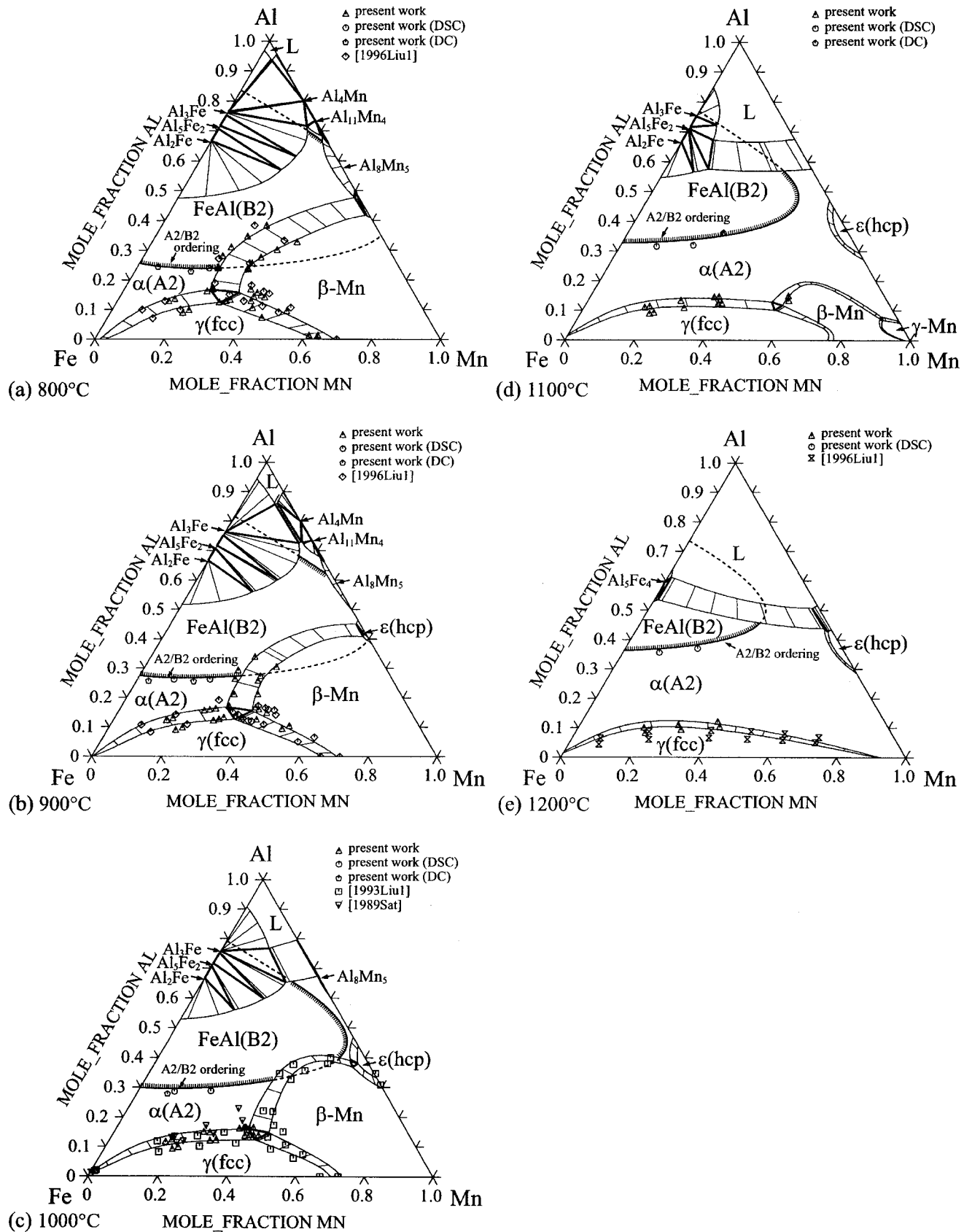


Fig. 3 Comparison between the calculated results and the experimental data at (a) 800 °C, (b) 900 °C, (c) 1000 °C, (d) 1100 °C, and (e) 1200 °C

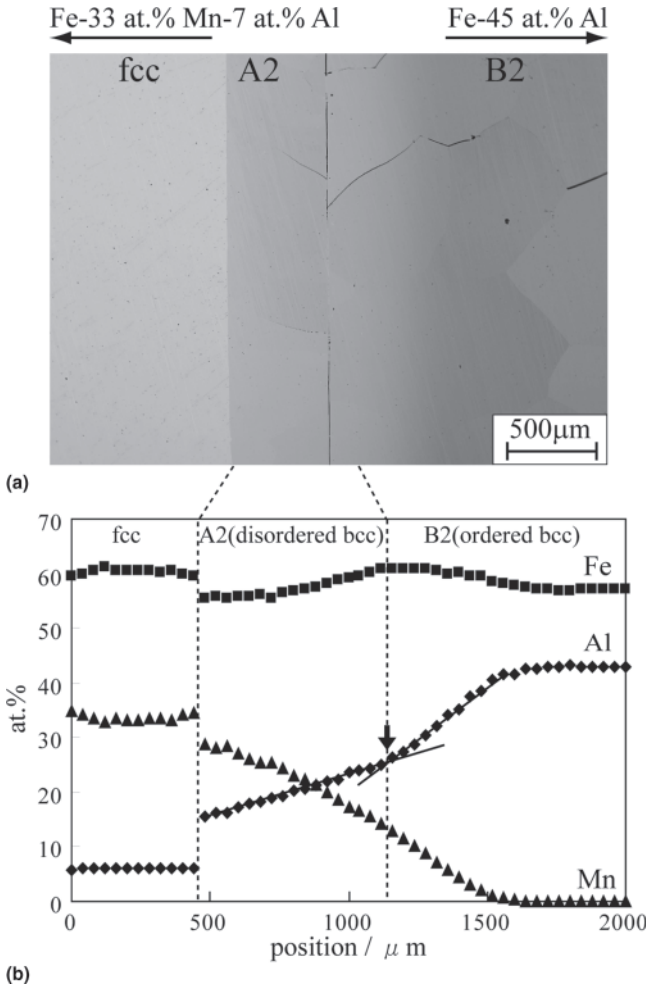


Fig. 4 (a) Backscattered electron image, and (b) the corresponding concentration in the Fe-33Mn-7Al/Fe-45Al diffusion couple annealed at 900 °C for 98 h (compositions in at.%)

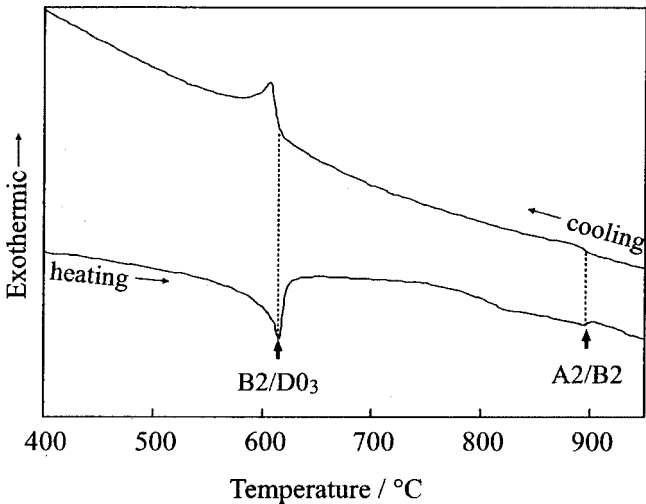


Fig. 5 DSC curve of the Fe-20Mn-27.5Al alloy at heating and cooling rates of 5 °C/min (compositions in at.%)

Table 2 Critical compositions of A2/B2 ordering transition determined by diffusion couple method

Temperature, °C	Critical compositions, at.%	
	A2/B2 ordering transition	
	Mn	Al
800	16.3	22.8
	6.0	24.4
900	16.6	25.5
	3.5	25.6
1000	8.8	27.8
1100	43.5	39.6

the Gibbs energy described by the compound energy formalism (CEF), where $G_m^{CEF}(y_i^{(s)})$, relates to $\Delta G_m^{ord}(y_i^{(s)})$:

$$\Delta G_m^{ord}(y_i^{(s)}) = G_m^{CEF}(y_i^{(s)}) - G_m^{CEF}(y_i^{(s)} = x_i) \quad (\text{Eq 4})$$

Here $y_i^{(s)}$ represents the site fraction of element i on the s th sublattice. $G_m^{CEF}(y_i^{(s)})$ is the molar Gibbs energy modeled with the two sublattice formalism, which consists of the order-dependent and the order-independent contributions and is described by the following equation:

$$G_m^{CEF}(y_i^{(s)}) = \sum_i \sum_j y_i^{(1)} y_j^{(2)} \circ G_{ij} + RT \left(\frac{1}{2} \sum_i y_i^{(1)} \ln y_i^{(1)} + \frac{1}{2} \sum_i y_i^{(2)} \ln y_i^{(2)} \right) + y_u^{(1)} y_v^{(1)} \sum_w y_w^{(2)} L_{u,v:w} + y_u^{(2)} y_v^{(2)} \sum_w y_w^{(1)} L_{w:u,v} \quad (\text{Eq 5})$$

In this equation, $i, j, u, v,$ and w represent any one of the ternary elements, Al, Fe and Mn, on condition that u is different from v and stands for the element prior to v in alphabetical order. $L_{u,v:w}$ and $L_{w:u,v}$ represent the interaction between u and v in the first and second sublattice, respectively, when another sublattice is occupied by w , and their composition dependence is described:

$$L_{u,v:w} = \sum_{m=0}^n {}^m L_{u,v:w} (y_u^{(1)} - y_v^{(1)})^m \quad \text{and} \\ L_{w:u,v} = \sum_{m=0}^n {}^m L_{w:u,v} (y_u^{(2)} - y_v^{(2)})^m \quad (\text{Eq 6})$$

All the ternary interactions in each sublattice and all the reciprocal interactions are not taken into account; i.e., values of these parameters are given as naught. $G_m^{CEF}(y_i^{(s)} = x_i)$ is the order independent contribution of $G_m^{CEF}(y_i^{(s)})$, which can be calculated on condition that all the site fractions of element i , $y_i^{(1)}$ and $y_i^{(2)}$ is equal to the composition of i , x_i . This term must be subtracted because the order independent contribution is taken into account by the subregular solution approximation shown by Eq 1. In this unified description,

Table 3 Critical temperatures determined by DSC

Composition, at. %	Mn-Al	A2/B2 ordering transition, °C	B2/D0 ₃ ordering transition, °C	Melting point, °C
10 Mn	10.6-24.0		590.0	...
	10.6-26.0	896.0	591.5	...
	10.8-29.0	1009.4	556.0	...
	10.6-33.6	1159.9	369.0	...
	10.6-38.6	1244.7
	10-50(a)	1274.0
	10-60(a)	1180.0
	10-70(a)	1087.0
	10-80(b)	1030.0
	10-90(b)	850.0
20 Mn	21.0-18.7	533.7
	20.9-23.6	782.0	609.9	...
	21.1-26.0	893.0	615.4	...
	21.1-28.7	986.1	590.1	...
	21.5-32.8	1130.1
	21.3-38.0	1210.0	...	1326.0
	20-50(a)	1227.5
	20-60(a)	1152.0
	20-70(a)	1053.0
	20-80(b)	970.0

(a) Nominal composition. (b) [1996Liu2]

thermodynamic properties and phase equilibria of the ordered and disordered phases can be evaluated separately.

The magnetic term is taken into account in the Gibbs energy of the bcc phase, which is described by Hillert and Jarl [1978Hil], as follows:

$$G_m^{\text{mag}} = RT(\beta + 1) \cdot f(\tau)$$

$$f(\tau) = 1 - \frac{1}{A} \cdot \left\{ \frac{79\tau^{-1}}{140p} + \frac{474}{497} \cdot \left(\frac{1}{p} - 1 \right) \cdot \left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600} \right) \right\}, \text{ for } \tau = \frac{T}{T_c} \leq 1$$

$$f(\tau) = -\frac{1}{A} \cdot \left(\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500} \right), \text{ for } \tau = \frac{T}{T_c} \geq 1$$

$$A = \frac{518}{1125} + \frac{11,692}{15,975} \cdot \left(\frac{1}{p} - 1 \right)$$

$$p = 0.40 \quad (\text{Eq 7})$$

where T_c is Curie temperature and β is magnetic moment.

3.3 Compound Phases

Because compound phases exist in the Fe-Al and Al-Mn binary systems, their Gibbs energies were expressed by the sublattice model; details of the thermodynamic models are described in [2004Ohn] and [1999Liu], respectively. The

lattice stabilities of the pure elements Fe, Al, and Mn were taken from Dinsdale [1991Din].

4. Results and Discussion

4.1 Experimental Determination

The typical fcc + bcc two-phase microstructure in the Fe-20Mn-10Al (at.%) alloy equilibrated at 800 °C for 336 h and the fcc + β Mn two-phase microstructure in the Fe-30Mn-30Al (at.%) alloy equilibrated at 900 °C for 98 h are shown in Fig. 2. The equilibrium compositions of the fcc, bcc, and β Mn phases from 800 to 1200 °C determined by EPMA are listed in Table 1, and the experimental data including the previous results [1996Liu1, 1993Liu1, 1989Sat] at 800, 900, 1000, 1100, and 1200 °C are plotted in Fig. 3. The present results on the isothermal sections at 800, 900, 1000, and 1200 °C are in good agreement with those reported by Liu et al. [1996Liu1, 1993Liu1]. However, the results of the fcc/bcc equilibrium at 1000 °C disagree with those reported by Sato et al. [1989Sat] because a considerable amount of C in their specimens affects the phase equilibria.

The diffusion couple method was used to determine the critical compositions of the A2/B2 ordering. Figure 4 shows a typical backscattered electron image and the corresponding concentration profiles in the Fe-33Mn-7Al/Fe-45Al (at.%) diffusion couple annealed at 900 °C. As shown in Fig. 4(b), the slope of the Al concentration sharply changes at a point indicated by an arrow. Such a singular point appearing in the concentration profile has been reported in

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Table 4 Summary of the thermodynamic parameters in the Fe-Mn-Al system

Phase	Thermodynamic parameter, J/mol	Phase	Thermodynamic parameter, J/mol
Liquid	${}^0L_{\text{Fe,Mn}}^{\text{Liq}}$	B2	${}^0G_{\text{Al:Al}}^{\text{B2}}$
	${}^1L_{\text{Fe,Mn}}^{\text{Liq}}$		${}^0G_{\text{Fe:Al}}^{\text{B2}}$
	${}^0L_{\text{Al,Mn}}^{\text{Liq}}$		${}^0G_{\text{Mn:Al}}^{\text{B2}}$
	${}^1L_{\text{Al,Mn}}^{\text{Liq}}$		${}^0G_{\text{Fe:Mn}}^{\text{B2}}$
	${}^2L_{\text{Al,Mn}}^{\text{Liq}}$		${}^0L_{\text{Al:Al,Fe}}^{\text{B2}}$
	${}^0L_{\text{Al,Fe}}^{\text{Liq}}$		${}^1L_{\text{Al,Fe:Al}}^{\text{B2}}$
	${}^1L_{\text{Al,Fe}}^{\text{Liq}}$		${}^0L_{\text{Al,Mn:Al}}^{\text{B2}}$
	${}^2L_{\text{Al,Fe}}^{\text{Liq}}$		${}^1L_{\text{Al,Mn:Al}}^{\text{B2}}$
	${}^0L_{\text{Al,Fe,Mn}}^{\text{Liq}}$		${}^0L_{\text{Fe,Mn:Al}}^{\text{B2}}$
	${}^0L_{\text{Fe,Mn}}^{\text{A2}}$		${}^1L_{\text{Fe,Mn:Al}}^{\text{B2}}$
	${}^0L_{\text{Al,Mn}}^{\text{A2}}$		${}^0L_{\text{Fe:Al,Fe}}^{\text{B2}}$
	${}^1L_{\text{Al,Mn}}^{\text{A2}}$		${}^1L_{\text{Al,Fe:Fe}}^{\text{B2}}$
	${}^0L_{\text{Al,Fe}}^{\text{A2}}$		${}^0L_{\text{Al,Mn:Fe}}^{\text{B2}}$
	${}^0T_{\text{cFe,Mn}}^{\text{A2}}$		${}^1L_{\text{Al,Mn:Fe}}^{\text{B2}}$
${}^0T_{\text{cAl,Fe}}^{\text{A2}}$	${}^0L_{\text{Al,Fe:Mn}}^{\text{B2}}$		
${}^1T_{\text{cAl,Fe}}^{\text{A2}}$	${}^1L_{\text{Al,Fe:Mn}}^{\text{B2}}$		
${}^1L_{\text{Al,Fe}}^{\text{A2}}$	${}^0L_{\text{Al,Mn:Mn}}^{\text{B2}}$		
${}^0L_{\text{Al,Mn}}^{\text{A12}}$	${}^1L_{\text{Al,Mn:Mn}}^{\text{B2}}$		
${}^0L_{\text{Al,Mn}}^{\text{A13}}$	${}^0T_{\text{cAl,Fe}}^{\text{B2}}$		
${}^0L_{\text{Fe,Mn}}^{\text{A13}}$	${}^0T_{\text{cAl,Mn}}^{\text{B2}}$		
${}^1L_{\text{Al,Mn}}^{\text{A13}}$	${}^0T_{\text{cAl,Fe:Al}}^{\text{B2}}$		
${}^0L_{\text{Al,Fe}}^{\text{A13}}$	${}^0T_{\text{cAl,Mn:Al}}^{\text{B2}}$		
${}^1L_{\text{Al,Fe}}^{\text{A13}}$	${}^0T_{\text{cFe:Al,Fe}}^{\text{B2}}$		
${}^0L_{\text{Al,Fe,Mn}}^{\text{A13}}$	${}^0T_{\text{cMn:Al,Fe}}^{\text{B2}}$		
${}^0L_{\text{Fe,Mn}}^{\text{A1}}$	${}^0T_{\text{cAl:Fe,Mn}}^{\text{B2}}$		
${}^1L_{\text{Fe,Mn}}^{\text{A1}}$	${}^0\beta_{\text{Al:Fe}}^{\text{B2}}$		
${}^0L_{\text{Al,Mn}}^{\text{A1}}$	${}^0\beta_{\text{Al:Mn}}^{\text{B2}}$		
${}^1L_{\text{Al,Mn}}^{\text{A1}}$	${}^0\beta_{\text{Al:Al,Fe}}^{\text{B2}}$		
${}^0L_{\text{Al,Fe}}^{\text{A1}}$	${}^0\beta_{\text{Al:Mn:Al}}^{\text{B2}}$		
${}^1L_{\text{Al,Fe}}^{\text{A1}}$	${}^0\beta_{\text{Al:Al,Mn}}^{\text{B2}}$		
${}^2L_{\text{Al,Fe}}^{\text{A1}}$	${}^0\beta_{\text{Al:Fe,Mn}}^{\text{B2}}$		
${}^0L_{\text{Al,Fe,Mn}}^{\text{A1}}$	${}^0\beta_{\text{Al:Fe:Fe}}^{\text{B2}}$		
${}^0T_{\text{cFe,Mn}}^{\text{A1}}$	${}^0\beta_{\text{Al:Mn:Fe}}^{\text{B2}}$		
${}^1T_{\text{cFe,Mn}}^{\text{A1}}$	${}^0\beta_{\text{Al,Fe:Mn}}^{\text{B2}}$		
${}^0L_{\text{Fe,Mn}}^{\text{hcp}}$	${}^0\beta_{\text{Mn:Al,Fe}}^{\text{B2}}$		
${}^1L_{\text{Fe,Mn}}^{\text{hcp}}$	${}^0\beta_{\text{Al,Mn:Mn}}^{\text{B2}}$		
${}^0L_{\text{Al,Mn}}^{\text{hcp}}$			
${}^1L_{\text{Al,Mn}}^{\text{hcp}}$			
${}^2L_{\text{Al,Mn}}^{\text{hcp}}$			
${}^0L_{\text{Al,Fe}}^{\text{hcp}}$			

many alloy systems such as Ni-Fe-Al [1984Hao], Co-Cr-Al [1998Ish], Ti-Al-Cr, and Ti-Al-Fe [2000Kai], and corresponds to the critical point of the A2/B2 ordering. The critical compositions of the A2/B2 order-disorder transition were thus determined with the compositions at the singular point. The critical compositions of the A2/B2 ordering are listed in Table 2.

Figure 5 shows a typical DSC curve for the Fe-21.1Mn-26.0Al (at.%) alloy, where $T_C^{\text{A2/B2}}$ and $T_C^{\text{B2/D0}_3}$ can be determined. The measured critical temperatures including A2/B2, B2/D0₃, and the melting point of the Fe-10Mn-Al and Fe-20Mn-Al (at.%) alloys are presented in Table 3, and their vertical sections are shown in Fig. 6. It is shown that

$T_C^{\text{A2/B2}}$ and $T_C^{\text{B2/D0}_3}$ increase with increasing Mn content in the composition range below 30 at.% Al. Figure 7 shows iso- $T_C^{\text{A2/B2}}$ contours of 800-1200 °C estimated from the present results.

4.2 Thermodynamic Calculation

The phase diagram of Fe-Al has been thermodynamically assessed by Allen et al. [1976Al11, 1976Al12]. Recently, Ohnuma et al. [2004Ohn] made a thermodynamic assessment of the Fe-Al system to describe the bcc ordering, including A2, B2, and D0₃ structures, using a four-sublattice model. In the present work, thermodynamic pa-

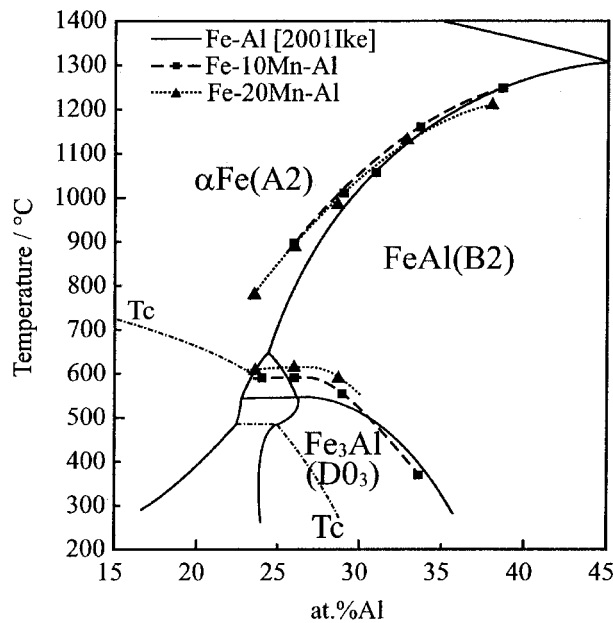


Fig. 6 Critical temperatures of the bcc ordering in the Fe-Mn-Al ternary system

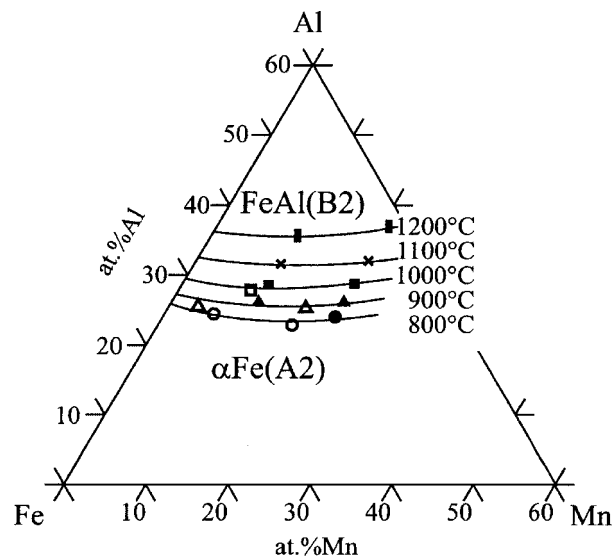


Fig. 7 Critical compositions of the A2/B2 ordering transition, determined by diffusion couple (open symbols) and DSC (closed symbols)

rameters of the A2 and B2 phases by Ohnuma et al. [2004Ohn] were used to describe the bcc ordering.

Jansson [1992Jan] carried out a thermodynamic assessment of the Al-Mn system. Subsequently, new experimental data including A2/B2 ordering were reported [1996Liu2]. Based on the experimental data, thermodynamic reassessment was conducted by Liu et al. [1999Liu], where the Gibbs energy of the bcc phase was described by the two-sublattice model. In the present work, the thermodynamic model of the bcc phase as reported by Liu et al. [1999Liu] was changed to the s-CEF model.

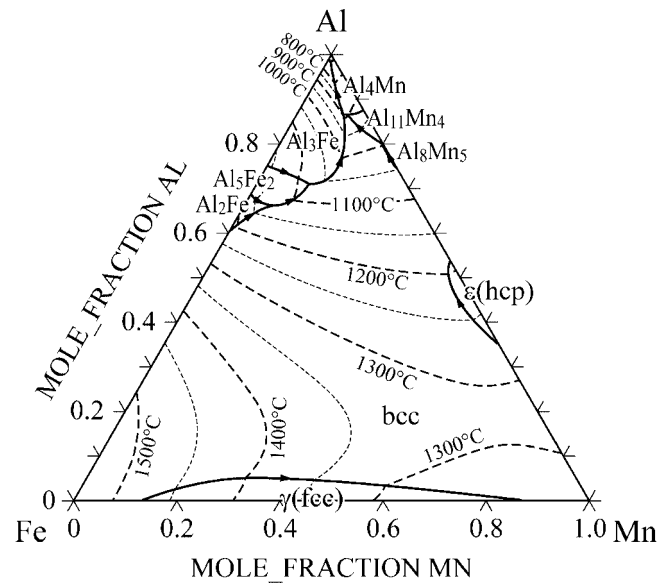


Fig. 8 Calculated liquidus surface in the Fe-Mn-Al system

In the present work, the thermodynamic parameters of the subsystems were taken from those of the Fe-Al [2004Ohn], Al-Mn [1999Liu], and Fe-Mn [1989Hua] binary systems.

Based on the present and previous experimental data, the thermodynamic parameters were evaluated using ThermoCalc software, which was originally developed by Sundman et al. [1985Sun]. The assessed parameters in the Fe-Mn-Al ternary system are listed in Table 4.

The thermodynamic parameters of the liquid, bcc, fcc, and β Mn phases were optimized by fitting the experimental data for liquidus lines and solid phase equilibria including A2/B2 ordering. Figure 3 shows a comparison of calculated isothermal sections with experimental data between 800 and 1200 °C. It is seen that good agreement is obtained between the calculated and experimental results. The calculated liquidus surface is also shown in Fig. 8.

5. Conclusions

The phase equilibria among the fcc, bcc, and β Mn phases and the critical temperatures of the A2/B2 and B2/DO₃ ordering in the Fe-Mn-Al ternary system were determined. It was found that the critical temperatures of ordering increase with increasing Mn content. Thermodynamic assessment of the Fe-Mn-Al system including A2/B2 ordering transition was carried out. The calculated results are in good agreement with the experimental data.

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Section I: Basic and Applied Research

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