Identification of Thermodynamically Stable Ceramic Reinforcement Materials for Iron Aluminide Matrices

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Aluminide-base intermetallic matrix composites are currently being considered as potential high-temperature materials. One of the key factors in the selection of a reinforcement material is its chemical stability in the matrix. In this study, chemical interactions between iron aluminides and several potential reinforcement materials, which include carbides, oxides, borides, and nitrides, are analyzed from thermodynamic considerations. Several chemically compatible reinforcement materials are identified for the iron aluminides with Al concentrations ranging from 40 to 50 at. pct.

I. INTRODUCTION

IRON aluminides are currently being considered as potential high-temperature structural materials. The iron-aluminum system, shown in Figure 1,[1] has an ordered α_2 phase with a B2 crystal structure and wide solubility limits. The alloys of current interest are within this α_2 phase with Al concentrations ranging from 40 to 50 at. pct. The alloy Fe-40Al* transforms to a disordered α

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*All alloy compositions are given in atomic percent.

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phase at about 1473 K. The melting temperature for the alloy Fe-50Al is about 1488 K. Thus, the upper use temperature limit for these two alloys would probably be about 1273 K. These alloys, in addition to having lower densities compared to the superalloys, have excellent cyclic oxidation resistance[2] up to 1273 K. Furthermore, the alloy Fe-40Al has exhibited good room-temperature ductility,[3] with elongation on the order of 3 to 5 pct. One potential drawback for the iron aluminides is their loss of strength above 700 K.[4] This can be overcome by reinforcing the aluminides with high-strength, high-modulus fibers. These fibers are, then, expected to carry the major portion of the load.

The reinforcement materials, besides having high strength and high modulus, must be chemically compatible with the matrices. For reinforcement materials that react excessively with the matrices, suitable coatings must be applied on the reinforcement materials. Prediction of chemical stabilities of different reinforcement materials in a given matrix, based on thermodynamic considerations, can narrow down the choices for reinforcement materials and thus reduce the experimental effort needed to identify potential reinforcement materials.

In this paper, the chemical interactions between iron aluminides and several potential reinforcement materials are analyzed from thermodynamic considerations. The primary aim of these analyses is to identify chemically compatible reinforcement materials for iron aluminide matrices with Al concentrations in the range of 40 to

50 at. pct. Keeping in mind the application temperature for the iron aluminides, all of the thermodynamic analyses were performed at 1273 K.

II. REINFORCEMENT MATERIALS

The reinforcement materials considered in this study included carbides, borides, oxides, and nitrides. A list of specific reinforcement materials considered in the present study is given in Table I. The reinforcement materials were chosen primarily because of their high melting points.

III. ACTIVITIES OF CONSTITUENT ELEMENTS IN THE INTERMETALLIC MATRIX

Reaction between the alloy and the reinforcement material would depend upon the activity of Fe and Al in the alloy. Radcliffe et al.[5] have measured the activity of Al (with respect to liquid Al) in Fe-Al alloys in the temperature range of 1148 to 1273 K by electromotive force measurements using a molten chloride electrolyte. The corresponding Fe activities were obtained by Gibbs-Duhem integration. The Al activities in Fe-Al alloys have also been measured by Eldridge and Komarek[6] by isopiestic method, and their activity data are in close agreement with those of Radcliffe et al.[5] The activity data of Radcliffe et al.[5] have been used in the present study. Table II gives the activities of Fe and Al in the FeAl phase as a function of Al concentration.

IV. IDENTIFICATION OF POSSIBLE PRODUCT COMPOUNDS

The first step in analyzing the chemical interactions between a reinforcement material and an intermetallic matrix is to identify pertinent chemical reactions. This, in turn, requires identification of possible product compounds that are stable in the matrix. Due to lack of thermodynamic data for ternary or higher order compounds, only binary product compounds will be considered in this study. The steps involved in identifying stable product compounds for a given reinforcement material–matrix combination are illustrated below for the FeAl-TiB$_2$ combination.
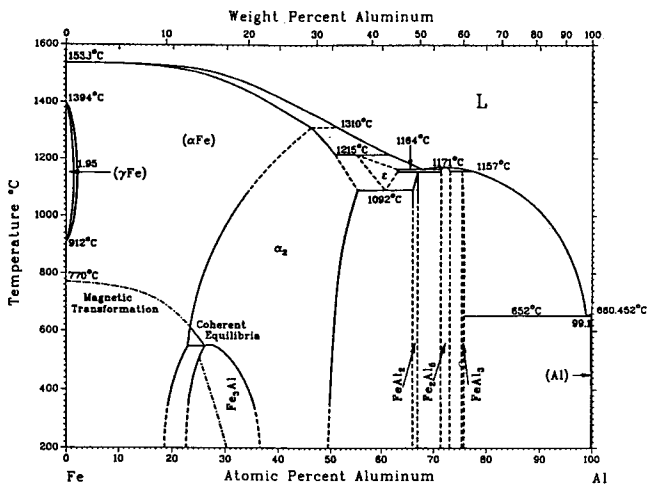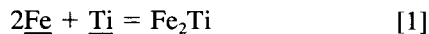

Fig. 1—Fe-Al phase diagram.[1]

The possible product compounds for the composite system FeAl-TiB$_2$ can be obtained by examining the phase diagrams for the four binary systems, Fe-Ti, Al-Ti, Fe-B, and Al-B. Two compounds, Fe$_2$Ti and FeTi, are possible in the binary Fe-Ti system. The formation of Fe$_2$Ti is governed by the equilibria for the reaction

$$2\underline{Fe} + \underline{Ti} = Fe_2Ti \qquad [1]$$

The underline in the above reaction indicates that the elements are present at reduced activities. The equilibrium constant for Reaction [1] can be expressed as

$$K_1 = 1/\{(a_{Fe})^2 * (a_{Ti})\} \qquad [2]$$

The activity product $(a_{Fe})^2 * (a_{Ti})$ must be greater than $1/K_1$ for Fe$_2$Ti to be formed inside the alloy. If we consider a situation in which the alloy is in contact with pure Ti (*i.e.*, the activity of Ti is unity), the activity of Fe in the alloy required for Fe$_2$Ti formation would be $(1/K_1)^{0.5}$. Clearly, if the activity of Fe in the alloy is less than $(1/K_1)^{0.5}$, Fe$_2$Ti cannot be formed even if the alloy is in contact with pure Ti. If this is the case, the compound Fe$_2$Ti need not be considered as a possible reaction product in our calculations.

The minimum activity of Fe in the alloy required for Fe$_2$Ti formation is calculated to be 0.046 at 1273 K, which

Table I. Reinforcement Materials Considered in This Study

Carbides	Borides	Oxides	Nitrides
B$_4$C	CrB$_2$	Al$_2$O$_3$	BN
HfC	HfB$_2$	BeO	HfN
SiC	LaB$_6$	CaO	LaN
TiC	ScB$_2$	CeO$_2$	Si$_3$N$_4$
ZrC	TiB$_2$	Cr$_2$O$_3$	TiN
	TiB	HfO$_2$	ZrN
	ZrB$_2$	La$_2$O$_3$	
		MgO	
		Sc$_2$O$_3$	
		SiO$_2$	
		TiO	
		TiO$_2$	
		Y$_2$O$_3$	

Table II. Activities of Iron* and Aluminum in FeAl Alloys at 1273 K**

Alloy Composition	a_{Fe}	a_{Al}
40	0.233	0.035
42	0.217	0.039
44	0.204	0.042
46	0.194	0.045
48	0.187	0.047
50	0.181	0.048

*Activity of Fe is with respect to bcc phase.
**Activity of Al is with respect to fcc Al.

is lower than the Fe activities in Fe-Al alloys within the concentration range of 40 to 50 at. pct Al. Therefore, Fe$_2$Ti should be considered as a possible reaction product. Calculations show that minimum conditions are also satisfied for the formation of FeTi. Between the two compounds Fe$_2$Ti and FeTi, only one compound needs to be considered. The stability of Fe$_2$Ti relative to that of FeTi is governed by the equilibria for the reaction

$$\underline{Fe} + FeTi = Fe_2Ti \qquad [3]$$

for which the equilibrium constant can be written as

$$K_3 = 1/(a_{Fe}) \qquad [4]$$

If the activity of Fe in the alloy is greater than $1/K_3$ (0.03 at 1273 K), Fe$_2$Ti would be the stable Fe-Ti compound. Since the activities of Fe in FeAl* alloys are greater

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*FeAl refers to Fe-Al alloys with Al concentrations in the range of 40 to 50 at. pct.

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than this value, Fe$_2$Ti will be considered to be the stable Fe-Ti compound in these alloys.

An examination of the binary system Al-Ti gives three possible product compounds: Ti$_3$Al, TiAl, and TiAl$_3$. For the Al concentrations in the range of 40 to 50 at. pct, the compound TiAl$_3$ cannot be formed even if the alloys are in contact with pure Ti. Between the two compounds Ti$_3$Al and TiAl, the latter one would be the stable Al-Ti compound inside the FeAl matrix.

The two possible Ti-containing product compounds that need to be considered for reaction of FeAl alloys with TiB$_2$ are Fe$_2$Ti and TiAl. The relative stability of these two compounds in the matrix are governed by the equilibria for the reaction

$$\underline{Al} + Fe_2Ti = TiAl + 2\underline{Fe} \qquad [5]$$
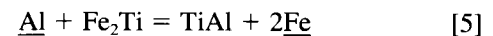
for which the equilibrium constant is written as

$$K_5 = (a_{Fe})^2/a_{Al} \qquad [6]$$

Thus, if the activity ratio $(a_{Fe})^2/(a_{Al})$ in the alloy is greater than K_5, then Fe$_2$Ti would be the stable compound in the FeAl alloy; otherwise, TiAl would be the stable product compound in the matrix. Calculations show that Fe$_2$Ti would be the stable product compound for FeAl alloys with Al concentrations in the range of 40 to 44 at. pct, whereas TiAl would be the stable product compound in the matrix for Al concentrations greater than 46 at. pct.

From the above considerations, it becomes apparent that only one Ti-containing product compound needs to be considered for reaction of an Fe-Al alloy with TiB$_2$.

Similarly, only one B-containing product compound needs to be considered. From thermodynamic calculations, the compound FeB would be the stable B-containing product compound in the FeAl matrices.

The stable reaction products in FeAl matrices for reaction with different elements of the reinforcement materials are shown in Table III. Thermodynamic data for all of the relevant intermetallic compounds except for Al-Zr, Fe-Zr, Al-Cr, Al-Hf, and Fe-Hf systems were obtained from standard compilations, including the *JANAF Thermochemical Tables*[7] and the compilations by Barin and Knacke.[8] The thermodynamic data for intermetallic compounds in the Al-Zr, Fe-Zr, and Al-Cr systems were obtained from the text by Hultgren *et al.*[9] The Gibbs energies of formation for Al-Hf and Fe-Hf compounds were assumed to be the same as the corresponding Al-Zr and Fe-Zr compounds.

The fact that the reaction products shown in Table III are stable in the matrix does not necessarily mean that these product compounds will be formed as a result of reaction of the matrix with the reinforcement materials. In order for these product compounds to be formed, the thermodynamics of the pertinent reactions must be favorable. This will be discussed in detail in the next section.

V. THERMODYNAMICS OF CHEMICAL INTERACTIONS BETWEEN IRON ALUMINIDES AND REINFORCEMENT MATERIALS

Chemical reaction between the reinforcement material and the intermetallic matrix can result in formation of reaction products at unit activity or at reduced activities. In a few cases, gaseous reaction products can also be formed. The chemical reactions are also likely to be influenced by any deviations from the stoichiometric composition for the reinforcement materials. Each of these situations will be discussed in detail in the following.

Table III. Stable Product Compounds in the Iron Aluminide Matrix for Different Elements of the Reinforcement Material

Element	Stable Product Compound
B	FeB
C	Al_4C_3
Ca	Al_2Ca
Ce	Al_2Ce
Cr	Al_6Cr_4
Hf	Al_2Hf
La	Al_2La
N	AlN
O	Al_2O_3
Sc	*
Si	FeSi
Ti	Fe_2Ti (<44 at. pct Al)
	TiAl (>46 at. pct Al)
Y	*
Zr	Al_2Zr

*Thermodynamic data not available for any product compounds containing these elements and Fe or Al.

A. Formation of Reaction Products at Unit Activity

Reinforcement material–matrix reactions in which reaction products are formed at unit activity can be divided into three categories. These are:

(1) direct reduction of the reinforcement material by an element of the intermetallic matrix;
(2) simultaneous formation of two product compounds as a result of the reaction of one element of the intermetallic matrix with the reinforcement material; and
(3) simultaneous formation of two product compounds as a result of the reaction of both the elements of the intermetallic matrix with the reinforcement material.

In the following, each of the above three modes of reactions will be discussed in detail with suitable examples drawn from each category.

1. *Direct reduction of the reinforcement material by an element of the intermetallic matrix*

One of the most straightforward reactions is direct reduction of the reinforcement material by an element of the intermetallic matrix in which an element of the reinforcement material is released. As an example of this, consider the reaction of FeAl alloys with B_4C. The reduction reaction resulting in formation of FeB and pure carbon is written as

$$4\underline{Fe} + B_4C = 4FeB + C \qquad [7]$$
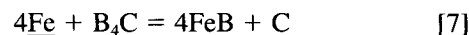
The first requirement for the above reaction to occur is that the standard Gibbs free energy change (ΔG°) for the reaction must be negative. However, a negative ΔG° for the reaction is not a sufficient condition for the reduction reaction to occur. The activity of Fe in the alloy must be greater than the equilibrium Fe activity for Reaction [7] in order for this reaction to go in the forward direction. From the equilibria expression for Reaction [7], the equilibrium activity of Fe is obtained to be $(1/K_7)^{1/4}$.

The ΔG° for Reaction [7] is negative, and the equilibrium activity of Fe for this reaction is $8.26 * 10^{-3}$. Since the activities of Fe in Fe-40Al (0.233) and in Fe-50Al (0.18) are greater than this equilibrium value, reaction of FeAl alloys with B_4C would result in the formation of FeB and pure carbon.

2. *Simultaneous formation of two product compounds by reaction of one element of the intermetallic matrix*

As an example of this, consider the reaction of FeAl alloys with ZrO_2. Thermodynamic calculations show that Al_2O_3 and Al_2Zr are the stable product compounds in the matrix. The ΔG° for the direct reduction reaction

$$4\underline{Al} \text{ (s)} + 3ZrO_2 = 2Al_2O_3 + 3Zr \qquad [8]$$

is positive (3.708 kcal) at 1273 K; thus, the above reaction is not feasible. Next, examine if the product compounds Al_2O_3 and Al_2Zr can be formed simultaneously by the reaction of ZrO_2 with the Al component of the matrix *via*

$$10\underline{Al} \text{ (s)} + 3ZrO_2 = 2Al_2O_3 + 3Al_2Zr \qquad [9]$$

The ΔG° for the above reaction must be negative in order for the reaction to take place. Furthermore, in order for Reaction [9] to occur, the activity of Al in the alloy must

be greater than the equilibrium Al activity for this reaction, which is calculated from the expression

$$K_9 = 1/(a_{Al})^{10} \qquad [10]$$

The ΔG° for Reaction [9] is negative at 1273 K, and the equilibrium Al activity for this reaction is $9.16 * 10^{-3}$. Since the activities of Al in Fe-40Al and Fe-50Al are greater than this value, FeAl alloys will react with ZrO_2 to form Al_2O_3 and Al_2Zr.

3. Simultaneous formation of two product compounds by reaction of both of the elements of the intermetallic matrix

Consider the reaction of FeAl alloys with SiC. The stable product compounds for the FeAl-SiC combination are FeSi and Al_4C_3. The ΔG° for the direct reduction reaction

$$4\underline{Al} \text{ (s)} + 3SiC = Al_4C_3 + 3Si \qquad [11]$$

is positive (3.02 kcal at 1273 K); therefore, this reaction is not feasible. The ΔG° for the other direct reduction reaction

$$\underline{Fe} + SiC = FeSi + C \qquad [12]$$
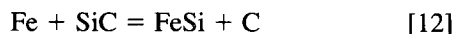
is negative (-3.03 kcal at 1273 K). However, the equilibrium Fe activity for this reaction is calculated to be 0.301, which is higher than the Fe activities in Fe-40 and 50 at. pct Al. Thus, Reaction [12] is not feasible for FeAl alloys.

Although both direct reduction reactions are not feasible, it is possible that the compounds Al_4C_3 and FeSi can be formed at the same time by simultaneous reaction of both components of the intermetallic matrix with SiC. The pertinent reaction is

$$3\underline{Fe} + 4\underline{Al} \text{ (s)} + 3SiC = 3FeSi + Al_4C_3 \qquad [13]$$
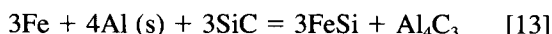
The ΔG° for this reaction is -46.96 kcal at 1273 K. Reaction [13] is feasible if the activity product $\{(a_{Fe})^3 * (a_{Al})^4\}$ in the alloy is greater than $1/K_{13}$, which is $8.64 * 10^{-9}$ at 1273 K. Since the activity products for both Fe-40Al ($1.89 * 10^{-8}$) and Fe-50Al ($3.14 * 10^{-8}$) are greater than this value, reaction of FeAl alloys with SiC would lead to formation of FeSi and Al_4C_3.

B. Formation of Reaction Products at Reduced Activity

Even though conditions are not favorable for formation of reaction products at unit activity, significant reaction can still occur by formation of reaction products at reduced activity. For example, consider the reaction of FeAl alloys with TiN. Thermodynamic calculations show that formation of product compounds at unit activity is not favorable for the FeAl-TiN combination. However, the products AlN and Ti can be formed at reduced activity via the reaction

$$\underline{Al} + TiN = \underline{AlN} + \underline{Ti} \qquad [14]$$
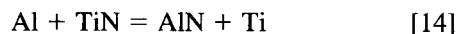
for which the equilibrium constant can be written as

$$K_{14} = \{(a_{AlN}) * (a_{Ti})\}/(a_{Al}) \qquad [15]$$

Even if the ΔG° for Reaction [14] is positive at 1273 K, this reaction will proceed in the forward direction by forming the reaction products at reduced activities; i.e., Ti would dissolve in the matrix, and AlN would dissolve in the reinforcement material. Reaction [14] will continue to proceed in the forward direction until the activity product $(a_{AlN})_{reinforcement} * (a_{Ti})_{matrix}$ becomes equal to $K_{14} * (a_{Al})$.

The equilibria for Reaction [14] gives the product of activities for the reaction products at equilibrium but not the individual activities. However, a minimum activity value for a reaction product can be calculated from the equilibria for Reaction [14] by assuming the activity of the other reaction product to be unity. Since the activities of AlN and Ti are related via Eq. [15], the calculation of the minimum value for the activity of one can give an indication of the magnitude of chemical interaction between the reinforcement material and the matrix. In our calculations, we prefer to report the minimum values for the activities of the elements of the reinforcement material in the intermetallic matrix.

The minimum value for the activity of Ti in the matrix for FeAl-TiN combination is calculated to be $1.32 * 10^{-3}$ and $1.82 * 10^{-3}$ for Fe-40Al and Fe-50Al, respectively. The actual amount of Ti dissolved in the FeAl matrix corresponding to these activity values would be a function of the ternary interaction coefficients in the Fe-Al-Ti system and cannot be predicted without thermodynamic data for the ternary solution. Since there is strong attractive interaction in the binary Fe-Ti and Al-Ti system, it is likely that the activity coefficient for Ti in the ternary Fe-Al-Ti system is quite low. Thus, an activity value on the order of 10^{-3} probably means that a significant amount of Ti would be dissolved in the FeAl matrix for the FeAl-TiN combination. For example, if the activity coefficient of Ti in the FeAl matrix is 0.1, then about 1 at. pct Ti would be dissolved in the FeAl matrix.

In a manner similar to those described above, the minimum value for the activity of N in the matrix can be calculated from the equilibria for the reactions:

$$\text{(for Fe-50Al)} \quad \underline{Al} + TiN = TiAl + \underline{N} \qquad [16]$$

$$\text{(for Fe-40Al)} \quad 2\underline{Fe} + TiN = Fe_2Ti + \underline{N} \qquad [17]$$

The calculated values for the minimum activities of N in the matrix are extremely low, being on the order of 10^{-24}. Thus, dissolution of N in the FeAl matrix for the FeAl-TiN combination would be insignificant and can be disregarded.

C. Formation of Gaseous Reaction Products

Gaseous reaction products can be formed if one constituent of the reinforcement material has a low boiling point. One such example is formation of gaseous Mg by reaction of FeAl alloys with MgO via

$$2\underline{Al} + 3MgO = Al_2O_3 + 3Mg \text{ (g)} \qquad [18]$$
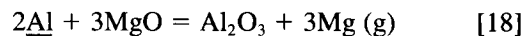
for which the equilibrium constant is

$$K_{18} \text{ (1273 K)} = 2.44 * 10^{-6} = (p_{Mg})^3/(a_{Al})^2 \qquad [19]$$

where p_{Mg} is the partial pressure of Mg. The equilibrium p_{Mg}'s for Fe-40Al and Fe-50Al are $1.45 * 10^{-3}$ and $1.7 *$

10^{-3} atm, respectively, at 1273 K. These partial pressures are considered to be relatively high, and if the matrix-reinforcement interface is exposed to a flowing gas environment, magnesium gas would be continuously swept away by the flowing gas, resulting in continuous conversion of MgO to Al_2O_3. However, if the MgO fibers are completely embedded in the matrix, the matrix-reinforcement interface would be quickly saturated with magnesium vapor, and the reaction would stop.

D. *Effect of Nonstoichiometry of the Reinforcement Material on Chemical Compatibility*

Consider the reaction of FeAl alloys with TiB_2. The compound TiB_2 exists over a narrow composition range from 65.5 to 67 at. pct B.[10] The activities of Ti and B can vary by many orders of magnitude over this composition range. For instance, based on the optimized thermodynamic data for the Ti-B system,[10] the Ti and B activities in TiB_2 at 1273 K corresponding to Ti-rich and B-rich boundaries are

Ti-rich boundary: $a_{Ti} = 1.737 * 10^{-4}$
$a_B = 5.48 * 10^{-5}$
B-rich boundary: $a_{Ti} = 5.22 * 10^{-13}$
$a_B = 1$

The Ti activity in TiB_2, even at the Ti-rich boundary, is lower than that required for formation of any Ti-containing reaction product (TiAl or Fe_2Ti) in FeAl matrices. Thus, no reaction between FeAl alloys and the Ti component of TiB_2 is likely to occur. On the other hand, the activity of B required for FeB formation in FeAl alloys is $8.89 * 10^{-3}$ for Fe-40Al and 0.011 for Fe-50Al. Thus, FeB can be formed by reaction of FeAl alloys with TiB_2 of higher B/Ti ratio, *i.e.*, for compositions closer to the B-rich boundary. However, since the range of homogeneity for TiB_2 is very narrow, any consumption of B by the reaction would shift the composition of TiB_2 toward the Ti-rich side, and the reaction would stop.

VI. RESULTS OF THERMODYNAMIC CALCULATIONS

Thermodynamic data for all of the ceramic reinforcement materials except for LaB_6 and ScB_2 were obtained from References 7 and 8. For these two compounds, only heat of formation data at 298 K were available.[11,12] The Gibbs energies of formation for these two compounds were assumed to be the same as the heat of formation at 298 K.

The reinforcement materials for which reaction products are formed at unit activity as a result of reaction with FeAl alloys are shown in Table IV. The pertinent chemical reactions are also shown in Table IV. It is probably safe to conclude that the reinforcement materials listed in Table IV would not be chemically compatible with FeAl alloys.

Table V gives the list of reinforcement materials for which the reaction products are likely to be formed at reduced activities. The calculated minimum values for the activities of the elements of the reinforcement material in the matrix are also shown in Table V. For FeAl-oxide and FeAl-nitride combinations, the minimum values for the activities of N and O in the matrix are very low and can be disregarded. These activity values are not shown in Table V.

Since no ternary or higher order compounds are considered in this study, the conclusion that the reinforcement materials listed in Table V would not react with the matrix to form reaction products at unit activity may not be always dependable. Experimental verification would be needed to confirm this. However, in general, it can be concluded that the lower the calculated minimum values for the activities of the elements of the reinforcement material in the matrix are, the greater would be the extent of chemical compatibility between the matrix and the reinforcement material. All of the reinforcement materials listed in Table V, except for TiN, would probably be chemically compatible with the FeAl alloys.

Of all of the reinforcement materials listed in Table I,

Table IV. List of Reinforcement Materials for Which Reaction Products Are Formed at Unit Activity and the Pertinent Reactions*

Ceramic Material	Chemical Reaction
B_4C	$4\underline{Fe} + B_4C = 4FeB + C$
Cr_2O_3	$2\underline{Al} + Cr_2O_3 = Al_2O_3 + 2Cr$
SiO_2	$4\underline{Al} + 3SiO_2 = 2Al_2O_3 + 3Si$
TiO_2	$4\underline{Al} + 3TiO_2 = 2Al_2O_3 + 3Ti$
BN	$\underline{Al} + BN = AlN + B$
Si_3N_4	$4\underline{Al} + Si_3N_4 = 4AlN + 3Si$
CrB_2	$6\underline{Al} + 8\underline{Fe} + 4CrB_2 = 8FeB + Al_6Cr_4$
SiC	$3\underline{Fe} + 4\underline{Al} + 3SiC = 3FeSi + Al_4C_3$
CaO	$8\underline{Al} + 3CaO = Al_2O_3 + 3CaAl_2$
CeO_2	$10\underline{Al} + 3CeO_2 = 2Al_2O_3 + 3Al_2Ce$
HfO_2	$10\underline{Al} + 3HfO_2 = 2Al_2O_3 + 3Al_2Hf$
TiO	$5\underline{Al} + 3TiO = Al_2O_3 + 3TiAl$ (for Fe-50Al)
	$6\underline{Fe} + 2\underline{Al} + 3TiO = Al_2O_3 + 3Fe_2Ti$ (for Fe-40Al)
ZrO_2	$10\underline{Al} + 3ZrO_2 = 2Al_2O_3 + 3Al_2Zr$
LaN	$3\underline{Al} + LaN = AlN + LaAl_2$
ZrN	$3\underline{Al} + ZrN = AlN + Al_2Zr$

*Unless otherwise stated, the reactions are valid for all alloy compositions within the range of 40 to 50 at. pct Al.

Table V. Minimum Values for the Equilibrium
Activities of the Elements of the Reinforcement Material
in the Matrix for Situations Where Reaction Products
Are Likely To Be Formed at Reduced Activities

Reinforcement Material	Minimum Equilibrium Activity Values in Fe-40Al	Minimum Equilibrium Activity Values in Fe-50Al
HfC	$a_{Hf} = 1.45 * 10^{-9}$ $a_C = 1.07 * 10^{-5}$	$a_{Hf} = 2.23 * 10^{-9}$ $a_C = 2.04 * 10^{-5}$
TiC	$a_{Ti} = 1.84 * 10^{-7}$ $a_C = 3.38 * 10^{-6}$	$a_{Ti} = 2.83 * 10^{-7}$ $a_C = 2.19 * 10^{-6}$
ZrC	$a_{Zr} = 4.29 * 10^{-8}$ $a_C = 3.16 * 10^{-4}$	$a_{Zr} = 6.59 * 10^{-8}$ $a_C = 6.04 * 10^{-4}$
HfB$_2$	$a_{Hf} = 1.05 * 10^{-9}$ $a_B = 2.93 * 10^{-6}$	$a_{Hf} = 6.37 * 10^{-10}$ $a_B = 4.06 * 10^{-5}$
LaB$_6$	$a_{La} = 1.34 * 10^{-4}$ $a_B = 4.4 * 10^{-3}$	$a_{La} = 2.95 * 10^{-5}$ $a_B = 4.91 * 10^{-3}$
ScB$_2$*	$a_{Sc} = 3.83 * 10^{-9}$ $a_B = 5.03 * 10^{-7}$	$a_{Sc} = 2.31 * 10^{-9}$ $a_B = 5.03 * 10^{-7}$
TiB$_2$	$a_{Ti} = 3.92 * 10^{-7}$ $a_B = 2.82 * 10^{-5}$	$a_{Ti} = 2.36 * 10^{-7}$ $a_B = 2.29 * 10^{-5}$
TiB	$a_{Ti} = 2.35 * 10^{-4}$ $a_B = 5.86 * 10^{-5}$	$a_{Ti} = 1.82 * 10^{-4}$ $a_B = 3.88 * 10^{-5}$
ZrB$_2$	$a_{Zr} = 7.45 * 10^{-9}$ $a_B = 7.8 * 10^{-5}$	$a_{Zr} = 4.49 * 10^{-9}$ $a_B = 1.08 * 10^{-4}$
BeO	$a_{Be} = 4.31 * 10^{-4}$	$a_{Be} = 5.34 * 10^{-4}$
La$_2$O$_3$	$a_{La} = 2.24 * 10^{-5}$	$a_{La} = 3.10 * 10^{-5}$
Sc$_2$O$_3$	$a_{Sc} = 2.15 * 10^{-7}$	$a_{Sc} = 2.97 * 10^{-7}$
Y$_2$O$_3$	$a_Y = 1.54 * 10^{-7}$	$a_Y = 2.12 * 10^{-7}$
HfN	$a_{Hf} = 2.68 * 10^{-5}$	$a_{Hf} = 3.7 * 10^{-5}$
TiN	$a_{Ti} = 1.32 * 10^{-3}$	$a_{Ti} = 1.82 * 10^{-3}$

*Minimum value for the activity of B obtained by assuming the activity of Sc to be unity.

Al$_2$O$_3$ would probably be the most stable reinforcement material in the iron aluminide matrices.

VII. SUMMARY AND CONCLUDING REMARKS

Reactions between iron aluminide matrices and ceramic reinforcement materials were analyzed from thermodynamic considerations, and several chemically compatible reinforcement materials were identified. These are: HfC, TiC, ZrC, HfB$_2$, ScB$_2$, TiB$_2$, ZrB$_2$, Al$_2$O$_3$, BeO, La$_2$O$_3$, Sc$_2$O$_3$, Y$_2$O$_3$, and HfN. For the ceramic materials which exist over a range of composition, the composition must be properly adjusted for optimum compatibility with the matrix.

One of the prime limitations of the thermodynamic calculations described in this paper is that ternary or higher order compounds are not considered. This is primarily due to lack of adequate data (thermodynamic as well as compositional) for ternary or higher order compounds. Clearly, the product compounds for a given composite system are likely to be different from those predicted in this study. However, this is less likely to change the final outcome of the calculations, which is to predict whether a given reinforcement material is likely to be compatible with the intermetallic matrix or not.

Because the reinforcement materials for the FeAl matrices are expected to carry a major portion of the load at high temperatures, a strong bond between the matrix and the reinforcement is required for effective load transfer. Thus, limited extent of chemical interaction at the matrix-reinforcement interface would be beneficial in this regard. The reactions that lead to formation of new compounds at the interface are probably not desirable because of the adverse effects of these compounds, which are normally brittle, on the mechanical properties of the composites. On the other hand, reactions in which a small amount of the reinforcement material is dissolved in the matrix might be beneficial for creating a strong bond between the matrix and the reinforcement material. Another approach would be to apply a thin layer of interfacial coating to promote a strong bond between the matrix and the reinforcement.

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