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Thermodynamic Analysis of Chemical Compatibility of Several Compounds With Fe-Cr-Al Alloys

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THERMODYNAMIC ANALYSIS OF CHEMICAL COMPATIBILITY OF SEVERAL COMPOUNDS WITH Fe-Cr-Al ALLOYS

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ABSTRACT

Chemical compatibility between Fe-19.8Cr-4.8Al (wt. %), which is the base composition for the commercial superalloy MA956, and several carbides, borides, nitrides, oxides, and silicides was analyzed from thermodynamic considerations. The effect of addition of minor alloying elements, such as Ti, Y, and Y_2O_3, to the FeCrAl alloy on chemical compatibility between the alloy and various compounds was also analyzed. Several chemically compatible compounds that can be potential reinforcement materials and/or interface coating materials for FeCrAl-based composites were identified.

INTRODUCTION

Alloys based on the ternary Fe-Cr-Al system are attractive as high temperature materials because of their excellent oxidation resistance, which is due to the formation of a protective Al_2O_3 scale during oxidation. Commercial Fe-Cr-Al-based alloys include Kanthal, widely used as resistance heating elements in high temperature furnaces, and MA956, which is used in heat exchanger tubes, combustion chambers, and burner nozzles.

Although alloys based on the ternary Fe-Cr-Al system have excellent oxidation resistant at high temperature, they possess low strengths at elevated temperatures. The high temperature strength of FeCrAl-based alloys can be improved by reinforcing them with strong, high-modulus fibers. One of the requirements in selecting a fiber composition is that the fiber be chemically compatible with the matrix. In case of chemically incompatible fiber-matrix combination, suitable interface reaction barrier layers are

needed. Interface coatings might also be required for other purposes which include: (1) protecting the fiber during processing, (2) optimizing the fiber-matrix bond, and (3) accommodating the residual stresses arising due to fiber-matrix coefficient of thermal expansion mismatch. When interface coatings are required, the coating composition must be chemically compatible with both the fiber and the matrix.

In this paper chemical interactions between alloys based on the ternary Fe-Cr-Al system and several compounds are analyzed from thermodynamic considerations. The primary objective of this study is to identify compounds that are chemically compatible with FeCrAl-based alloys. These compounds may then be more fully explored for their effectiveness as reinforcement materials or interface coatings. The general approach is similar to that reported in earlier papers by this author which addressed the chemical compatibility of different reinforcement materials with nickel aluminides (ref. 1) and iron aluminides (ref. 2).

ALLOY AND COMPOUNDS STUDIED

The alloy composition considered in this study is Fe-19.8Cr-4.8Al (in wt. %)[1], which is nearly the same as that of the commercial superalloy MA956 (Fe-20Cr-4.5Al-0.5Ti-0.5Y_2O_3). This composition was selected because of the availability of thermodynamic data for this ternary alloy. The effect of addition (about 0.5 %) of minor alloying elements such as Ti, Y, and Y_2O_3 on chemical compatibility of the various compounds with Fe-19.8Cr-4.8Al is also considered in this study

Table I gives a list of compounds considered in this study. The list includes carbides, borides, oxides, nitrides, and silicides. The compounds in Table I were chosen primarily because of their high melting points.

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[1] Unless otherwise stated, the alloy compositions are in weight percent.

THERMODYNAMIC DATA

Chemical compatibility calculations on fiber-matrix or coating-matrix interactions require (refs. 1 and 2) data on activity of constituent elements in the matrix and the Gibbs energy of formation (ΔG_f°) of the compounds. Hilpert and Miller (ref. 3) have investigated the vaporization of Fe-19.8Cr-4.8Al alloy in the temperature range 1313 to 1554 K by Knudsen effusion mass spectrometry, and have obtained equilibrium partial pressures of Fe,Cr, and Al over this alloy as a function of temperature. Knowing the equilibrium partial pressure of elements over the alloy, the activities of Fe, Cr, and Al in the alloy can be calculated from the expression

$$a_i = p_i/p_i^\circ \qquad [1]$$

where a_i is the activity of element i (i = Fe, Cr, or Al), p_i is the equilibrium partial pressure of species i over the alloy, and p_i° is the equilibrium vapor pressure of pure i. The activities of different elements in Fe-19.8Cr-4.8Al at 1400 and 1500 K are shown in Table II.

The activity of Ti in superalloys containing a small amount of Ti (0.5 to 1 wt. %) is in the range of 10^{-3} to 10^{-5} at 1300 K (ref. 4). The effect of a small amount of Ti in the matrix on the chemical compatibility of different compounds with Fe-19.8Cr-4.8Al is calculated for two Ti activities: 10^{-3} and 10^{-5}. Similar activity values are also used to calculate the effect of Y addition on chemical compatibility.

The ΔG_f° of different compounds were obtained from Janaf Thermochemical Tables (ref. 5), and from compilations by Barin and Knacke (ref. 6) and Barin (ref. 7). The ΔG_f° for a few relevant intermetallic compounds were taken from other sources, which are referenced in two previous publications (refs. 1 and 2).

METHOD OF CALCULATION

The calculation procedures are similar to those described in previous papers (refs. 1 and 2). The calculations, in general, consist of two steps. First, all possible reaction

product compounds that may result from each matrix-compound pairing are identified. The next step consists of writing the possible reactions between the alloy matrix and a potential reinforcement or coating compound, and determining the thermodynamic feasibility for the reactions. The sequence of steps necessary to determine the compatibility of a given compound with the matrix is outlined in figure 1.

Identification of stable reaction products in the matrix

The procedure to identify the stable product compound is described here for the reaction of Fe-19.8Cr-4.8Al with a boride. Reaction of FeCrAl with the boron component of the boride can result in several product compounds, such as Fe-B, Cr-B, or Al-B compounds. Because of a lack of thermodynamic data for ternary compounds, only binary product compounds are considered in this study. Several possible B-containing compounds that need to be considered are FeB, Fe_2B, CrB, CrB_2, AlB_2, and AlB_{12}. However, only one B-containing product compound will be stable in Fe-19.8Cr-4.8Al, and only this compound needs to be considered in the thermodynamic analysis.

The stable B-containing compound in the Fe-19.8Cr-4.8Al matrix is determined by an iterative process which considers the stability of one compound relative to the other. Consider the two Cr-B compounds, CrB and CrB_2. The relative stabilities of CrB and CrB_2 are governed by the equilibria for reaction

$$CrB_2 + Cr = 2CrB \qquad [1]$$

The equilibrium activity of Cr (a_{Cr}) for reaction [1] at 1500 K is 4.09×10^{-3}, which means that if a_{Cr} in the matrix is greater than 1.98×10^{-3}, CrB will be the stable Cr-B compound in the matrix. Because a_{Cr} in Fe-19.8Cr-4.8Al at 1500 K is 0.28 ($> 4.09 \times 10^{-3}$), CrB_2 can be eliminated as a possible reaction product. Similar calculations eliminate Fe_2B and AlB_{12} as possible reaction products.

Now, among the three possible B-containing reaction products, FeB, CrB, and AlB_2, only one will be stable in the Fe-19.8Cr-4.8Al matrix. The relative stabilities of FeB

and CrB in Fe-19.8Cr-4.8Al are governed by the equilibria for the reaction

$$FeB + Cr = CrB + Fe \qquad [2]$$

The equilibrium activity ratio (a_{Fe}/a_{Cr}) for Reaction [2] at 1500 K is 5.406. Thus, the activity ratio (a_{Fe}/a_{Cr}) in the alloy at 1500 K must be less than 5.406 for CrB to be stable; otherwise FeB will be stable relative to CrB_2. The activity ratio (a_{Fe}/a_{Cr}) in the Fe-19.8Cr-4.8Al alloy at 1500 K is 2.351, which is less than 5.406. Therefore, among the compounds CrB and FeB, CrB will be relatively stable in the matrix.

Next, consider the relative stabilities of CrB and AlB_2 in the Fe-19.8Cr-4.8Al alloy, which is governed by the equilibria for the reaction

$$2CrB + \underline{Al} = AlB_2 + 2\underline{Cr} \qquad [3]$$

At 1500 K the activity ratio (a_{Cr}^2/a_{Al}) in the alloy must be less than 4.75×10^{-2} for AlB_2 to be stable relative to CrB_2. The activity ratio (a_{Cr}^2/a_{Al}) in the alloy at 1500 K is 26.13, which is much greater than 4.75×10^{-2}. Thus, among CrB and AlB_2, CrB will be relatively stable in the Fe-19.8Cr-4.8Al alloy. Because CrB is also relatively stable in the alloy with respect to FeB, CrB will be the stable B-containing compound in the Fe-19.8Cr-4.8Al alloy. Therefore, CrB is considered as a possible product for analyzing the feasibility of reaction of Fe-19.8Cr-4.8Al with any boride.

Similar calculations give Cr_7C_3 as the possible reaction product for reaction of Fe-19.8Cr-4.8Al with carbides, AlN for reaction with nitrides, and Al_2O_3 for reaction with oxides. The possible product compound for reaction of Fe-19.8Cr-4.8Al with silicides can be either FeSi or Cr_5Si_3, depending on the thermodynamic data used. Use of thermodynamic data from the compilations by Barin and Knacke (ref. 6) gives FeSi to be the possible product compound, whereas use of data from the compilations by Barin (ref. 7) gives Cr_5Si_3 to be the stable product compound. In this paper, chemical compatibility of silicides with Fe-19.8Cr-4.8Al is examined assuming Cr_5Si_3 as the stable product compound in the matrix. Although it is equally likely that FeSi can be the stable product

compound, the conclusions derived with the assumption of Cr_5Si_3 as the stable product compound are not likely to change.

Examination of chemical interactions between FeCrAl and different compounds

Once reaction products are identified, the thermodynamic feasibility of different possible reactions is examined. The types of reactions, as described in the previous papers (refs. 1 and 2), are (1) direct reduction of the compound by an element of the matrix, (2) simultaneous formation of two product compounds, and (3) formation of products at reduced activities, i.e., at activities less than unity. These reaction types are discussed below, using as examples, B_4C, BN, and TiB_2.

One of the most straightforward reactions is direct reduction of the reinforcement/coating compound by an element of the alloy matrix in which an element of the reinforcement/coating compound is released. Consider the reaction of Fe-19.8Cr-4.8Al with B_4C. The reduction reaction of Fe-19.8Cr-4.8Al with B_4C resulting in formation of CrB and pure carbon is written as

$$4\underline{Cr} + B_4C = 4CrB + C \qquad [4]$$

where the underline denotes a reduced activity, i.e., activity less than unity for the element or the compound. The first requirement for Reaction [4] 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 Cr in the alloy must be greater than the equilibrium Cr activity for this reaction to occur. The equilibrium a_{Cr} for Reaction [4] at 1400 K is 2.54×10^{-3}, which is lower than the a_{Cr} (0.33) in the alloy. Therefore, Fe-19.8Cr-4.8Al will react with B_4C at 1400 K to form CrB and free carbon, and therefore B_4C is not chemically compatible with this alloy.

If a direct reduction reaction, as described above, is not thermodynamically feasible, the next step is to consider the feasibility of formation of two product compounds simultaneously. An example is reaction of Fe-19.8Cr-4.8Al with BN. For the direct

reduction reaction

$$\underline{Al} + BN = AlN + B \qquad [5]$$

to occur at 1400 K, the a_{Al} in the alloy must be greater than 0.043, which is an order of magnitude lower than the a_{Al} in the alloy ($2.6x10^{-3}$). Thus, AlN and B cannot form by Reaction [5]. Next, consider the formation of both AlN and CrB by the reaction

$$\underline{Al} + \underline{Cr} + BN = AlN + CrB \qquad [6]$$

The ΔG° for Reaction [6] must be negative and the activity product ($a_{Cr}*a_{Al}$) in the alloy must be greater than the equilibrium activity product $(a_{Cr}*a_{Al})_{eq.}$ for Reaction [6] to occur. The ΔG° for Reaction [6] is -28.75 kCal and the $(a_{Cr}*a_{Al})_{eq.}$ for this reaction is $3.28x10^{-5}$ at 1400 K. Because the ($a_{Cr}*a_{Al}$) in the alloy at 1400 K, $8.58x10^{-4}$, is greater than the $(a_{Cr}*a_{Al})_{eq}$ for Reaction [6], both AlN and CrB will form by this reaction. Therefore, BN is not chemically compatible with Fe-19.8Cr-4.8Al.

Even if both direct reduction reaction, and reaction where two compounds can form simultaneously at unit activity, are not thermodynamically feasible, reaction between the alloy and any potential fiber/coating compound can still occur by forming reaction products at reduced activities (activities less than unity). Consider the reaction of Fe-19.8Cr-4.8Al with TiB_2. Because CrB is the stable product compound in the matrix, the reaction can be written as

$$2\underline{Cr} + TiB_2 = 2CrB + \underline{Ti} \qquad [7]$$

The equilibrium Ti activity for Reaction [7] corresponding to the a_{Cr} in the alloy is $1.15x10^{-6}$ at 1400 K, which is quite low. Assuming ideal solution behavior for Ti in the alloy, an activity of $1.5x10^{-6}$ corresponds to dissolution of 1.5 ppm of Ti in the alloy due to the reaction. The amount of Ti dissolved in the alloy will be somewhat higher if there is strong interaction between Ti and other components of the alloy. For example, if the activity coefficient of Ti in the alloy is 0.01, then 150 ppm of Ti will dissolve in the alloy as a result of reaction with TiB_2. Such levels of Ti in the alloy is probably acceptable.

There can be another possible reaction of Fe-19.8Cr-4.8Al with TiB_2, resulting in formation of both CrB_2 and Ti at reduced activities. As mentioned earlier, among CrB and CrB_2, CrB will be the stable reaction product in the matrix. This is only true if CrB_2 forms at unit activity. The compound CrB_2 can be the stable reaction product in the matrix if it can form at a reduced activity, e.g., by dissolving in the reacting boride. The equilibrium activity of CrB_2 for Reaction [1] at 1400 K is 8.8×10^{-3}; therefore, CrB_2 can be the stable reaction product if its activity is less than 8.8×10^{-3}.

Reaction of the Fe-19.8Cr-4.8Al alloy with TiB_2 resulting in formation of CrB_2 and Ti, both at reduced activities, can be written as

$$\underline{Cr} + TiB_2 = \underline{CrB_2} + \underline{Ti} \qquad [8]$$

The equilibrium activity product ($a_{CrB2} * a_{Ti}$) for Reaction [8] at 1400 K is 3.087×10^{-8}. Assuming ideal solution behavior for TiB_2-CrB_2 and FeCrAl-Ti systems, and from mass balance considerations, the equilibrium mole fractions of CrB_2 in TiB_2 and of Ti in the alloy at 1400 K are both equal to 1.01×10^{-4}. This means about 100 ppm of CrB_2 will dissolve in TiB_2 and about the same amount of Ti will dissolve in the alloy due to reaction of Fe-19.8Cr-4.8Al with TiB_2. These dissolved amounts will be higher if negative deviations from ideality are considered for both the TiB_2-CrB_2 and FeCrAl-Ti systems. Again, the amounts of CrB_2 dissolved in TiB_2 and of Ti dissolved in the alloy are probably small enough to cause any adverse effects on the composite properties. Thus, TiB_2 can be considered to be chemically compatible with Fe-19.8Cr-4.8Al.

When the reaction products form at activities less than unity, the extent of reaction is a function of the equilibrium activity of the reaction products; the lower the equilibrium activities for the reaction products, the greater will be the extent of chemical compatibility between the alloy and the fiber/coating compound. For situations where reaction products form at reduced activities, determination of whether a compound is chemically compatible with the alloy matrix is rather subjective. However, for screening purposes, the

compound can be considered to be chemically compatible with the alloy if the activities of the reaction products are less than 10^{-3}. If the activities of the reaction products are between 10^{-3} and 10^{-2}, the compatibility of the compound with the alloy is reported as "borderline ".

RESULTS OF THERMODYNAMIC CALCULATIONS FOR THE Fe-Cr-Al ALLOY

Tables III to VII give the possible reaction products for reaction of Fe-19.8Cr-4.8Al with carbides, nitrides, borides, oxides, and silicides, respectively. The results are reported for two different temperatures, 1400 and 1500 K, which correspond to potential use temperature and processing temperature for FeCrAl-based composites, respectively.

A list of compounds that are likely to be chemically compatible with Fe-19.8Cr-4.8Al is given in Table VIII. Note that there are several compounds that are likely to be chemically compatible with Fe-19.8Cr-4.8Al.

EFFECT OF Ti IN THE ALLOY ON CHEMICAL COMPATIBILITY

The compounds that are likely to be chemically compatible with Fe-19.8Cr-4.8Al (given in Table VIII) were further screened for their chemical compatibility with an alloy containing 0.5 % Ti. Two examples are given below to describe the effect of 0.5 % Ti on the chemical compatibility of compounds with the Fe-19.8Cr-4.8Al alloy.

Consider the effect of Ti on the chemical compatibility of CrB with the Fe-19.8Cr-4.8Al alloy. The reaction between the Ti component of the alloy and CrB can be written as

$$\underline{Ti} + 2CrB = TiB_2 + Cr \qquad [9]$$

For an a_{Cr} of 0.33 at 1400 K, the equilibrium Ti activity for Reaction [9] at 1400 K is 1.15×10^{-6}. If the Ti activity in the alloy is greater than 1.15×10^{-6}, TiB_2 will form by Reaction [9]. For 0.5 % Ti in the alloy, the activity of Ti is in the range of 10^{-3} to 10^{-5}; therefore, CrB will not be stable in an alloy containing 0.5 % Ti.

As another example, consider reaction of HfB_2 with a Fe-19.8Cr-4.8Al-0.5Ti alloy.

From the equilibria for the reaction

$$\underline{Ti} + HfB_2 = TiB_2 + Hf \qquad [10]$$

the equilibrium a_{Hf} at 1400 K is 1.99×10^{-4} for an a_{Ti} of 10^{-3} and 1.99×10^{-6} for an a_{Ti} of 10^{-5}. Because these Hf activities are quite low, HfB_2 can be considered to be chemically compatible with the Fe-19.8Cr-4.8-0.5Ti alloy.

A list of compounds that are likely to be chemically compatible with the Fe-19.8Cr-4.8Al-0.5Ti alloy is shown in Table IX.

EFFECT OF Y_2O_3 IN THE ALLOY ON CHEMICAL COMPATIBILITY (Chemical compatibility of compounds with MA956)

In addition to a small amount of Ti, the commercial alloy MA956 contains about 0.5 % Y_2O_3. Yttrium oxide will not affect the chemical compatibility of carbides, borides, nitrides, and silicides with the Fe-19.8Cr-4.8Al-0.5Ti alloy. However, Y_2O_3 reacts with many oxides, as seen from the phase diagrams of various oxides with Y_2O_3 (refs. 8 and 9). Thus, many of the oxides shown in Table IX will not be chemically compatible with a FeCrAl alloy containing Y_2O_3. Table X shows a list of compounds that are likely to be chemically compatible with the alloy MA956.

Some commercial FeCrAl-based alloys contain a small amount of Y instead of Y_2O_3. Yttrium will again affect chemical compatibility of the oxides with the alloy. Because of the very high stability of Y_2O_3, the Y component of the alloy will invariably react with almost any oxide to form Y_2O_3. Even Y_2O_3-containing compounds such as $Y_3Al_5O_{12}$ (YAG) will not be chemically compatible with alloys containing Y because of the reaction of Y with the Al_2O_3 component of YAG

$$2\underline{Y} + Al_2O_3 = Y_2O_3 + 2\underline{Al} \qquad [11]$$

EFFECT OF COMPOUND NONSTOICHIOMETRY ON CHEMICAL COMPATIBILITY

Many compounds exhibit deviations from the stoichiometric composition; i.e., they can exist over a narrow composition range. One such example is TiB_2 which can exist over a composition range from 65.5 to 67 at. pct. B (ref. 10). The activities of Ti and B

can vary by many orders of magnitude over this composition range. For instance, based on optimized thermodynamic data for the Ti-B system (ref. 10), the activities of Ti and B at 1400 K at Ti-rich and B-rich boundaries are

Ti-rich boundary: $a_{Ti} = 6.73 \times 10^{-4}$

$a_B = 1.79 \times 10^{-5}$

B-rich boundary: $a_{Ti} = 8.13 \times 10^{-12}$

$a_B = 1$

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, such as Fe_2Ti or TiAl, in the Fe-19.8Cr-4.8Al matrix. On the other hand, CrB can form in the Fe-19.8Cr-4.8Al alloy at 1400 K for a boron activity of 2.24×10^{-3}. Thus, for TiB_2 composition closer to the B-rich boundary, CrB can form by reaction of the alloy with TiB_2. However, since the range of homogeneity for TiB_2 is very narrow, any consumption of B by the reaction will shift the composition of TiB_2 toward the Ti-rich side, and the reaction will stop. Thus, some reaction between TiB_2 and the alloy might be expected if the TiB_2 is B-rich, but the extent of reaction is likely to be minimal. This small extent of reaction might be beneficial for obtaining a good bond at the matrix-fiber or the matrix-coating interface. Many borides exhibit similar nonstoichiometry, and the conclusions derived for TiB_2 are equally valid for other borides.

Another nonstoichiometric compound is ZrO_2, which can exist as oxygen-deficient ZrO_2, i.e., as ZrO_{2-x} (ref. 9). Thus, if stoichiometric ZrO_2 is the starting composition for the fiber or the coating, ZrO_2 can react with the alloy to form alumina by the reaction

$$ZrO_2 + (2x/3)\underline{Al} = ZrO_{2-x} + (x/3)Al_2O_3 \qquad [12]$$

Again, the reaction will progress only to a limited extent, because consumption of oxygen by Reaction [12] will shift the composition of ZrO_2 toward the Zr-rich boundary after which the reaction will stop. It is plausible that this small extent of reaction might be desirable for getting a better bonding at the matrix-coating or the matrix-fiber interface.

INTERFACE COATING COMPOSITIONS FOR MA956/Al_2O_3 COMPOSITE

Single crystal (c-axis) Al_2O_3 fibers are being considered as potential reinforcement materials for the MA956 matrix. As discussed, Al_2O_3, although thermodynamically stable in Fe-Cr-Al alloys, is not chemically compatible with MA956 because the alloy contains Y_2O_3. Thus, suitable interface reaction barriers are required for a MA956/Al_2O_3 composite. Suitable interface reaction barrier compositions were identified by examining the chemical compatibility of compounds listed in Table X (i.e., compounds likely to be chemically compatible with MA956) with Al_2O_3. All the borides, carbides, nitrides, and silicides listed in Table X are chemically compatible with Al_2O_3.

On the other hand, all the oxides listed in Table X are likely to react with Al_2O_3 to form compound oxides. However, one compound oxide $Y_3Al_5O_{12}$ (YAG) can still be a potential interface coating composition. YAG is chemically compatible with Al_2O_3 but will react with Y_2O_3 to form $Y_4Al_2O_9$ (ref. 9). However, because of only a small amount of Y_2O_3 in the alloy, it is likely that a thin outer layer of the YAG coating will react with the surrounding Y_2O_3 in the alloy and thus deplete the alloy of Y_2O_3 in the interface region, after which the reaction will stop.

If the composite is processed by powder metallurgy techniques, it is likely that the internal particles in the alloy are YAG instead of Y_2O_3, which is due to reaction of Y_2O_3 with the trace amount of Al_2O_3 in the MA956 powder. If this is the case, YAG will be chemically compatible with the alloy containing Y_2O_3.

Table XI provides a list of potential interface coating compositions, that are likely to be chemically compatible with both MA956 and Al_2O_3. The compositions listed in Table XI are based on chemical compatibility considerations only; any interface coating must also meet the mechanical requirements, a discussion of which is beyond the scope of this paper.

SUMMARY AND CONCLUDING REMARKS

Reaction between Fe-19.8Cr-4.8Al, with and without minor addition of other alloying elements such as Ti and Y_2O_3, with several carbides, borides, nitrides, oxides, and silicides was analyzed from thermodynamic considerations. From these analyses, several chemically compatible compounds that can be potential reinforcement materials and/or interface coating materials for FeCrAl-based composites have been identified. In addition, potential interface coating compositions for the MA956/Al_2O_3 composite have been identified. A few compounds have been identified whose compatibility with the Fe-Cr-Al alloy might be "borderline", i.e., they may or maynot be chemically reactive with the alloy. These "borderline" compounds might offer some advantages with regard to improving the fiber-matrix or the matrix-coating bond, if a strong bond is desired at either of these interfaces.

One of the prime limitations of the thermodynamic calculations reported in this paper is that ternary or higher order compounds are not considered as possible reaction products. This is primarily due to lack of adequate data, thermodynamic as well as compositional, for ternary or higher order compounds. Thus, the product compounds for a given combination 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 compound is likely to be compatible with the alloy.

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Table I. Compounds considered in compatibility calculations

Carbides	Borides	Oxides	Nitrides	Silicides
Al_4C_3	AlB_{12}	Al_2O_3	AlN	Cr_3Si
B_4C	CrB_2	BeO	BN	Cr_5Si_3
$Cr_{23}C_6$	HfB_2	CaO	HfN	Mo_3Si
Cr_7C_3	LaB_6	CeO_2	LaN	Mo_5Si_3
Cr_3C_2	NbB_2	Cr_2O_3	Si_3N_4	$MoSi_2$
HfC	ScB_2	Gd_2O_3	TaN	Nb_5Si_3
Mo_2C	TaB_2	HfO_2	TiN	$NbSi_2$
Nb_2C	TiB_2	La_2O_3	ZrN	Ta_2Si
NbC	TiB	MgO		Ta_5Si_3
SiC	VB	Sc_2O_3		$TaSi_2$
TaC	VB_2	SiO_2		Ti_5Si_3
Ta_2C	V_3B_2	TiO		TiSi
TiC	V_2B_3	TiO_2		$TiSi_2$
V_2C	ZrB_2	Y_2O_3		V_3Si
VC		ZrO_2		$V_{5Si}3$
W_2C		Ca_2SiO_4		VSi_2
WC		$CaZrO_3$		W_5Si_3
ZrC		$Y_2O_3.ZrO_2$		WSi_2
		$Y_3Al_5O_{12}$		Zr_2Si
		(YAG)		Zr_5Si_3
		$Y_4Al_2O_9$		ZrSi

TABLE II. Activities of Fe, Cr, and Al in Fe-19.8Cr-4.8Al alloy

Temperature (K)	Activity of Fe	Activity of Cr	Activity of Al
1400	0.52	0.33	2.6×10^{-3}
1500	0.48	0.28	3×10^{-3}

TABLE III. Reaction of Fe-19.8Cr-4.8Al with carbides
(undeline in a reaction denotes activities less than unity)

Carbide	Reaction product
Al_4C_3	Cr_7C_3 stable product in matrix
B_4C	$4\underline{Cr} + B_4C = 4CrB + C$
$Cr_{23}C_6$	Cr_7C_3 stable product in matrix
Cr_3C_2	Cr_7C_3 stable product in matrix
HfC	$7\underline{Cr} + 3HfC = Cr_7C_3 + 3\underline{Hf}$
	$(a_{Hf})_{eq.} = 2.6\times10^{-8}$ at 1400 K
	$= 5.48\times10^{-8}$ at 1500 K
Mo_2C	$7\underline{Cr} + 3Mo_2C = Cr_7C_3 + 6\underline{Mo}$
	$(a_{Mo})_{eq.} = 0.36$ at 1400 K
	$= 0.3$ at 1500 K
NbC	$6\underline{Fe} + 7\underline{Cr} + 3NbC = Cr_7C_3 + 3Fe_2Nb$ (1400 K)
	(conditions just sufficient at 1400 K)
	$7\underline{Cr} + 3NbC = Cr_7C_3 + 3\underline{Nb}$
	$(a_{Nb})_{eq.} = 3.09\times10^{-4}$ at 1500 K
Nb_2C	$12\underline{Fe} + 7\underline{Cr} + 3Nb_2C = Cr_7C_3 + 3Fe_2Nb$
SiC	$5\underline{Cr} + 3SiC = Cr_5Si_3 + 3C$
TaC	$7\underline{Cr} + 3TaC = Cr_7C_3 + 3\underline{Ta}$
	$(a_{Ta})_{eq.} = 1.48\times10^{-4}$ at 1400 K
	$= 1.7\times10^{-4}$ at 1500 K
Ta_2C	$7\underline{Cr} + 3Ta_2C = Cr_7C_3 + 6\underline{Ta}$
	$(a_{Ta})_{eq.} = 6.43\times10^{-4}$ at 1400 K
	$= 8.39\times10^{-4}$ at 1500 K

Table III (contd.). Reaction of Fe-19.8Cr-4.8Al with carbides
(Underline denotes activities less than unity)

Carbide	Reaction product
TiC	$7\underline{Cr} + 3TiC = Cr_7C_3 + 3\underline{Ti}$
	$(a_{Ti})_{eq.} = 1.43 \times 10^{-5}$ at 1400 K
	$= 2.16 \times 10^{-5}$ at 1500 K
V_2C	$7\underline{Cr} + 3V_2C = Cr_7C_3 + 6\underline{V}$
	$(a_V)_{eq.} = 0.067$ at 1400 K
	$= 0.068$ at 1500 K
VC	$7\underline{Cr} + 3VC = Cr_7C_3 + 3\underline{V}$
	$(a_V)_{eq.} = 0.011$ at 1400 K
	$= 0.011$ at 1500 K
W_2C	$7\underline{Cr} + 3W_2C = Cr_7C_3 + 6W$
WC	$7\underline{Cr} + 3WC = Cr_7C_3 + 3W$ at 1400 K
	$7\underline{Cr} + 3WC = Cr_7C_3 + 3\underline{W}$ at 1500 K
	$(a_W)_{eq.} = 0.83$ at 1500 K
ZrC	$7\underline{Cr} + 3ZrC = Cr_7C_3 + 3\underline{Zr}$
	$(a_{Zr})_{eq.} = 3.33 \times 10^{-6}$ at 1400 K
	$= 5.25 \times 10^{-6}$ at 1500 K

Table IV. Reaction of Fe-19.8Cr-4.8Al with borides
(Undeline denotes species present at activities less than unity)

Boride	Reaction product
AlB_{12}	CrB stable reaction product in matrix
CrB_2	CrB stable reaction product in matrix
HfB_2	$2\underline{Cr} + HfB_2 = 2CrB + \underline{Hf}$
	$(a_{Hf})_{eq.} = 2.3x10^{-7}$ at 1400 K
	$= 4.76x10^{-7}$ at 1500 K
	$\underline{Cr} + HfB_2 = \underline{CrB_2} + \underline{Hf}$
	Ideal solution: $a_{CrB2} = a_{Hf} = 7.8x10^{-5}$ at 1400K
	$a_{CrB2} = a_{Hf} = 1.58x10^{-4}$ at 1500 K
NbB_2	$2\underline{Fe} + 2\underline{Cr} + NbB_2 = 2CrB + Fe_2Nb$
	(conditions just sufficient fo this reaction)
ScB_2	$2\underline{Cr} + ScB_2 = 2CrB + \underline{Sc}$
	$(a_{Sc})_{eq.} = 6.92x10^{-7}$ at 1400 K
	$= 1.22x10^{-6}$ at 1500 K
	$\underline{Cr} + ScB_2 = \underline{CrB_2} + \underline{Sc}$
	Ideal solution: $a_{CrB2} = a_{Sc} = 1.36x10^{-4}$ (1400 K)
	$= 2.52x10^{-4}$ (1500 K)
TaB_2	$2\underline{Cr} + TaB_2 = 2CrB + \underline{Ta}$
	$(a_{Ta})_{eq.} = 9.79x10^{-3}$ at 1400 K
	$= 9.88x10^{-3}$ at 1500 K
TiB_2	$2\underline{Cr} + TiB_2 = 2CrB + \underline{Ti}$
	$(a_{Ti})_{eq.} = 1.15x10^{-6}$ at 1400 K
	$= 2.37x10^{-6}$ at 1500 K
	$\underline{Cr} + TiB_2 = \underline{CrB_2} + \underline{Ti}$
	Ideal solution: $a_{CrB2} = a_{Ti} = 1x10^{-4}$ (1400 K)
	$= 3.5x10^{-4}$ (1500 K)

Table IV. (contd.) Reaction of Fe-19.8Cr-4.8Al with borides
(Underline denotes species at activities less than unity)

Boride	Reaction product
TiB	$\underline{Cr} + TiB = CrB + \underline{Ti}$
	$(a_{Ti})_{eq.} = 7.95 \times 10^{-4}$ at 1400 K
	$= 1.15 \times 10^{-3}$ at 1500 K
	$\underline{Cr} + TiB = \underline{CrB} + \underline{Ti}$
	Ideal solution: $a_{CrB} = a_{Ti} = 0.05$ (1400 K)
VB	$\underline{Cr} + VB = CrB + \underline{V}$
	$(a_V)_{eq.} = 5.78 \times 10^{-3}$ at 1400 K
	$= 7.07 \times 10^{-3}$ at 1500 K
VB_2	$2\underline{Cr} + VB_2 = 2CrB + \underline{V}$
	$(a_V)_{eq.} = 0.017$ at 1400 K
	$= 0.017$ at 1500 K
V_3B_2	$2\underline{Cr} + V_3B_2 = 2CrB + 3\underline{V}$
	$(a_V)_{eq.} = 0.015$ at 1400 K
	$(a_V)_{eq.} = 0.018$ at 1500 K
V_2B_3	$3\underline{Cr} + V_2B_3 = 3CrB + 2\underline{V}$
	$(a_V)_{eq.} = 8.92 \times 10^{-3}$ at 1400 K
	$= 9.82 \times 10^{-3}$ at 1500 K
ZrB_2	$2\underline{Cr} + ZrB_2 + 2CrB + \underline{Zr}$
	$(a_{Zr})_{eq.} = 1.7 \times 10^{-6}$ at 1400 K
	$= 3.5 \times 10^{-6}$ at 1500 K
	$\underline{Cr} + ZrB_2 = \underline{CrB_2} + \underline{Zr}$
	Ideal solution: $a_{CrB2} = a_{Zr} = 2.1 \times 10^{-4}$ (1400 K)
	$= 4.3 \times 10^{-4}$ (1500 K)

Table V. Reaction of Fe-19.8Cr-4.8Al with nitrides
(Underline denotes activities less than unity)

Nitride	Reaction
AlN	No reaction
BN	$\underline{Al} + \underline{Cr} + BN = AlN + CrB$
HfN	$\underline{Al} + HfN = AlN + \underline{Hf}$
	$(a_{Hf})_{eq.} = 1.8\times10^{-6}$ at 1400 K
	$= 2.5\times10^{-6}$ at 1500 K
LaN	$\underline{Al} + LaN = AlN + \underline{La}$
	$(a_{La})_{eq.} = 0.01$ at 1400 K
	$= 0.01$ at 1500 K
Si_3N_4	$4\underline{Al} + Si_3N_4 = 4AlN + 3Si$
TaN	$\underline{Al} + TaN = AlN + \underline{Ta}$
	$(a_{Ta})_{eq.} = 0.05$ at 1400 K
	$= 0.035$ at 1500 K
Ta_2N	$\underline{Al} + Ta_2N = AlN + 2\underline{Ta}$
	$(a_{Ta})_{eq.} = 0.17$ at 1400 K
	$= 0.15$ at 1500 K
TiN	$\underline{Al} + TiN = AlN + \underline{Ti}$
	$(a_{Ti})_{eq.} = 7.49\times10^{-5}$ at 1400 K
	$= 9.01\times10^{-5}$ at 1500 K
	$\underline{Al} + TiN = \underline{AlN} + \underline{Ti}$
	Ideal solution: $a_{AlN} = a_{Ti} = 8.65\times10^{-3}$ at 1400 K
	$a_{AlN} = a_{Ti} = 9.5\times10^{-3}$ at 1500 K
ZrN	$\underline{Al} + ZrN = AlN + \underline{Zr}$
	$(a_{Zr})_{eq.} = 6.72\times10^{-6}$ at 1400 K
	$= 9.45\times10^{-6}$ at 1500 K
	$\underline{Al} + ZrN = \underline{AlN} + \underline{Zr}$
	Ideal solution: $a_{AlN} = a_{Zr} = 2.6\times10^{-3}$ at 1400 K
	$a_{AlN} = a_{Zr} = 3.07\times10^{-3}$ at 1500 K

Table VI. Reaction of Fe-19.8Cr-4.8Al with oxides
(Underline denotes activities less than unity)

Oxide	Reaction
Al_2O_3	No reaction
BeO	$2\underline{Al} + 3BeO = Al_2O_3 + 3\underline{Be}$
	$(a_{Be})_{eq.} = 8.71\times10^{-5}$ at 1400 K
	$= 1.22\times10^{-5}$ at 1500 K
CaO	$2\underline{Al} + 3CaO = Al_2O_3 + 3\underline{Ca}$
	$(a_{Ca})_{eq.} = 2.03\times10^{-5}$ at 1400 K
	$= 3.5\times10^{-5}$ at 1500 K
	$2\underline{Al} + 4CaO = CaAl_2O_4 + 3\underline{Ca}$
	$(a_{Ca})_{eq.} = 6.59\times10^{-5}$ at 1400 K
	$= 1.08\times10^{-4}$ at 1500 K
CeO_2	$4\underline{Al} + 3CeO_2 = 2Al_2O_3 + 3\underline{Ce}$
	$(a_{Ce})_{eq..} = 1.67\times10^{-3}$ at 1400 K
	$= 1.67\times10^{-3}$ at 1500 K
Ce_2O_3	$2\underline{Al} + Ce_2O_3 = Al_2O_3 + 2\underline{Ce}$
	$(a_{Ce})_{eq.} = 3.7\times10^{-7}$ at 1400 K
	$= 6.1\times10^{-7}$ at 1500 K
Cr_2O_3	Al_2O_3 stable oxide
Gd_2O_3	$2\underline{Al} + Gd_2O_3 = Al_2O_3 + 2\underline{Gd}$
	$(a_{Gd})_{eq.} = 8.14\times10^{-7}$ at 1400 K
	$= 1.31\times10^{-6}$ at 1500 K
HfO_2	$4\underline{Al} + 3HfO_2 = 2Al_2O_3 + 3\underline{Hf}$
	$(a_{Hf})_{eq.} = 9.72\times10^{-6}$ at 1400 K
	$= 1.01\times10^{-5}$ at 1500 K
La_2O_3	$2\underline{Al} + La_2O_3 = Al_2O_3 + 2\underline{La}$
	$(a_{La})_{eq.} = 1.94\times10^{-6}$ at 1400 K
	$= 3.03\times10^{-6}$ at 1500 K

Table VI. (contd.) Reaction of Fe-19.8Cr-4.8Al with oxides
(Underline denotes activities less than unity)

MgO	$2\underline{Al} + 3MgO = Al_2O_3 + 3\underline{Mg}$
	$(a_{Mg})_{eq.} = 7.48 \times 10^{-4}$ at 1400 K
	$2\underline{Al} + 3MgO = Al_2O_3 + 3Mg(g)$
	$(p_{Mg})_{eq.} = 8.96 \times 10^{-4}$ at 1400 K
	$= 2.62 \times 10^{-3}$ at 1500 K
Sc_2O_3	$2\underline{Al} + Sc_2O_3 = Al_2O_3 + 2\underline{Sc}$
	$(a_{Sc})_{eq.} = 2.78 \times 10^{-8}$ at 1400 K
	$= 5.87 \times 10^{-8}$ at 1500 K
SiO_2	$4\underline{Al} + 3SiO_2 = 2Al_2O_3 + 3Si$
TiO	$2\underline{Al} + 3TiO = Al_2O_3 + 3\underline{Ti}$
	$(a_{Ti})_{eq.} = 0.017$ at 1400 K
	$= 0.016$ at 1500 K
TiO_2	$4\underline{Al} + 3TiO_2 = 2Al_2O_3 + 3Ti$
Y_2O_3	$2\underline{Al} + Y_2O_3 = Al_2O_3 + 2\underline{Y}$
	$(a_Y)_{eq.} = 1.92 \times 10^{-8}$ at 1400 K
	$= 3.95 \times 10^{-8}$ at 1500 K
ZrO_2	$4\underline{Al} + 3ZrO_2 = 2Al_2O_3 + 3\underline{Zr}$
	$(a_{Zr})_{eq.} = 1.03 \times 10^{-4}$ at 1400 K
	$= 1.02 \times 10^{-4}$ at 1500 K
Ca_2SiO_4	$4\underline{Al} + 3\underline{SiO_2} = 2Al_2O_3 + 3Si$
$CaZrO_3$	CaO-rich: $(a_{ZrO2}) = 0.036$
	$4\underline{Al} + 3\underline{ZrO_2} = 2Al_2O_3 + 3\underline{Zr}$
	$(a_{Zr})_{eq.} = 3.72 \times 10^{-6}$ at 1400 K
	$= 4.54 \times 10^{-6}$ at 1500 K
	ZrO_2-rich -- same as pure ZrO_2
$Y_2O_3.ZrO_2$	similar to that of ZrO_2
$Y_3Al_5O_{12}$	Similar to that of Y_2O_3

Table VII. Reaction of Fe-19.8Cr-4.8Al with silicides
(Underline denotes activities less than unity)

Silicide	Reaction
Cr_3Si	Cr_5Si_3 stable reaction product in matrix
Cr_5Si_3	No reaction
Mo_3Si	$5\underline{Cr} + 3Mo_3Si = Cr_5Si_3 + 9\underline{Mo}$
	$(a_{Mo})_{eq.}$ = 0.81 at 1400 K
	= 0.73 at 1500 K
Mo_5Si_3	$5\underline{Cr} + Mo_5Si_3 = Cr_5Si_3 + 5\underline{Mo}$
	$(a_{Mo})_{eq.}$ = 0.37 at 1400 K
	= 0.30 at 1500 K
$MoSi_2$	$10\underline{Cr} + 3MoSi_2 = 2Cr_5Si_3 + 3\underline{Mo}$
	$(a_{Mo})_{eq.}$ = 0.05 at 1400 K
	= 0.06 at 1500 K
Nb_5Si_3	$5\underline{Cr} + 10\underline{Fe} + Nb_5Si_3 = Cr_5Si_3 + 5Fe_2Nb$
$NbSi_2$	$10\underline{Cr} + 3NbSi_2 = 2Cr_5Si_3 + 3Nb$
Ta_2Si	$5\underline{Cr} + 3Ta_2Si = Cr_5Si_3 + 6\underline{Ta}$
	$(a_{Ta})_{eq.}$ = 0.21 at 1400 K
	= 0.19 at 1500 K
Ta_5Si_3	$5\underline{Cr} + Ta_5Si_3 = Cr_5Si_3 + 5\underline{Ta}$
	$(a_{Ta})_{eq.}$ = 0.29 at 1400 K
	= 0.25 at 1500 K
$TaSi_2$	$10\underline{Cr} + 3TaSi_2 = 2Cr_5Si_3 + 3Ta$
Ti_5Si_3	$5\underline{Cr} + Ti_5Si_3 = Cr_5Si_3 + 5\underline{Ti}$
	$(a_{Ti})_{eq.}$ = 5.08×10^{-3} at 1400 K
	= 5.88×10^{-3} at 1500 K
TiSi	$5\underline{Cr} + 3TiSi = Cr_5Si_3 + 3\underline{Ti}$
	$(a_{Ti})_{eq.}$ = 0.05 at 1400 K
	= 0.04 at 1500 K
$TiSi_2$	$10\underline{Cr} + 3TiSi_2 = 2Cr_5Si_3 + 3Ti$

Table VII. (contd.) Reaction of Fe-19.8Cr-4.8Al with silicides
(Underline denotes activities less than unity)

Silicide	Reaction
V_3Si	$5\underline{Cr} + 3V_3Si = Cr_5Si_3 + 9\underline{V}$
	$(a_V)_{eq.} = 0.63$ at 1400 K
	$= 0.58$ at 1500 K
V_5Si_3	$5\underline{Cr} + V_5Si_3 = Cr_5Si_3 + 5\underline{V}$
	$(a_V)_{eq.} = 0.015$ at 1400 K
	$= 0.014$ at 1400 K
VSi_2	$10\underline{Cr} + 3VSi_2 = 2Cr_5Si_3 + 3\underline{V}$
	$(a_V)_{eq.} = 0.096$ at 1400 K
	$= 0.107$ at 1500 K
W_5Si_3	$5\underline{Cr} + W_5Si^3 = Cr_5Si_3 + 5W$
WSi_2	$10\underline{Cr} + 3WSi_2 = 2Cr_5Si_3 + 3W$
Zr_5Si_3	$5\underline{Cr} + Zr_5Si_3 = Cr_5Si_3 + 5\underline{Zr}$
	$(a_{Zr})_{eq.} = 5.7\times10^{-3}$ at 1400 K
	$= 6.68\times10^{-3}$ at 1500 K
$ZrSi_2$	$10\underline{Cr} + 3ZrSi_2 = 2Cr_5Si_3 + 3Zr$
Zr_2Si	$5\underline{Cr} + 3Zr_2Si = Cr_5Si_3 + 6\underline{Zr}$
	$(a_{Zr})_{eq.} = 6.78\times10^{-3}$ at 1400 K
	$= 8.13\times10^{-3}$ at 1500 K
ZrSi	$5\underline{Cr} + 3ZrSi = Cr_5Si_3 + 3\underline{Zr}$
	$(a_{Zr})_{eq.} = 6.34\times10^{-3}$ at 1400 K
	$= 6.52\times10^{-3}$ at 1500 K

Table VIII. Compounds likely to be chemically compatible with Fe-19.8Cr-4.8Al (at both 1400 and 1500 K)

Carbides	Borides	Nitrides	Oxides	Silicides
Cr_7C_3	CrB	AlN	Al_2O_3	Cr_5Si_3 **
HfC	HfB_2	HfN	BeO	Ti_5Si_3 **
NbC*	ScB_2	TiN*	CaO	Zr_5Si_3 **
TaC	TiB_2	ZrN	CeO_2*	Zr_2Si **
Ta_2C	TiB*		Ce_2O_3	ZrSi **
TiC	ZrB_2		Gd_2O_3	
			HfO_2	
			La_2O_3	
			MgO	
			Sc_2O_3	
			Y_2O_3	
			ZrO_2	
			$CaZrO_3$	
			$Y_2O_3.ZrO_2$	
			$Y_3Al_5O_{12}$ (YAG)	
			$Y_4Al_2O_9$	

---

* Borderline case

** Need experimental verification due to uncertainty in thermodynamic data.

Table IX. Compounds likely to be chemically compatible with Fe-19.8Cr-4.8Al-0.5Ti (at both 1400 and 1500 K)

Carbides	Borides	Nitrides	Oxides	Silicides
Cr_7C_3*	HfB_2	AlN*	Al_2O_3	Cr_5Si_3 **
HfC	ScB_2	TiN	BeO	Ti_5Si_3 **
Ta_2C*	TiB_2	HfN	CaO	Zr_5Si_3 **
TiC	TiB*	ZrN	CeO_2*	Zr_2Si **
ZrC	ZrB_2		Ce_2O_3	ZrSi **
			Gd_2O_3	
			HfO_2	
			La_2O_3	
			MgO	
			Sc_2O_3	
			Y_2O_3	
			ZrO_2	
			$CaZrO_3$	
			$Y_2O_3.ZrO_2$	
			$Y_3Al_5O_{12}$ (YAG)	
			$Y_4Al_2O_9$	

Table X. Compounds likely to be chemically compatible with alloy MA956 (alloy composition close to Fe-19.8Cr-4.8Al-0.5Ti-0.5Y_2O_3) (at both 1400 and 1500 K)

Carbides	Borides	Nitrides	Oxides	Silicides
Cr_7C_3 *	HfB_2	AlN*	BeO	Cr_5Si_3 **
HfC	ScB_2	TiN	CaO	Ti_5Si_3 **
Ta_2C*	TiB_2	HfN	MgO	Zr_5Si_3 **
TiC	TiB*	ZrN	Y_2O_3	Zr_2Si **
ZrC	ZrB_2		Y_2O_3-ZrO_2	ZrSi **
			$Y_4Al_2O_9$	

---

* Borderline case

** Need experimental verification due to uncertainty in thermodynamic data.

Other oxides, such as Ce_2O_3, and Gd_2O_3, might be compatible if they do not react with Y_2O_3.

Table XI. Interface coating compositions that are chemically compatible with bot MA956 and Al_2O_3 at 1400 and 1500 K

Carbides	Borides	Nitrides	Oxides	Silicides
Cr_7C_3 *	HfB_2	AlN*	$Y_3Al_5O_{12}$ ***	Cr_5Si_3 **
HfC	ScB_2	TiN	(YAG)	Ti_5Si_3 **
Ta_2C*	TiB_2	HfN		Zr_5Si_3 **
TiC	TiB*	ZrN		Zr_2Si **
ZrC	ZrB_2			ZrSi **

---

* Borderline case

** Need experimental verification due to uncertainty in thermodynamic data.

*** The oxide compound $Y_3Al_5O_{12}$ (YAG) might be a possible interface coating because of kinetic reasons discussed in the text.

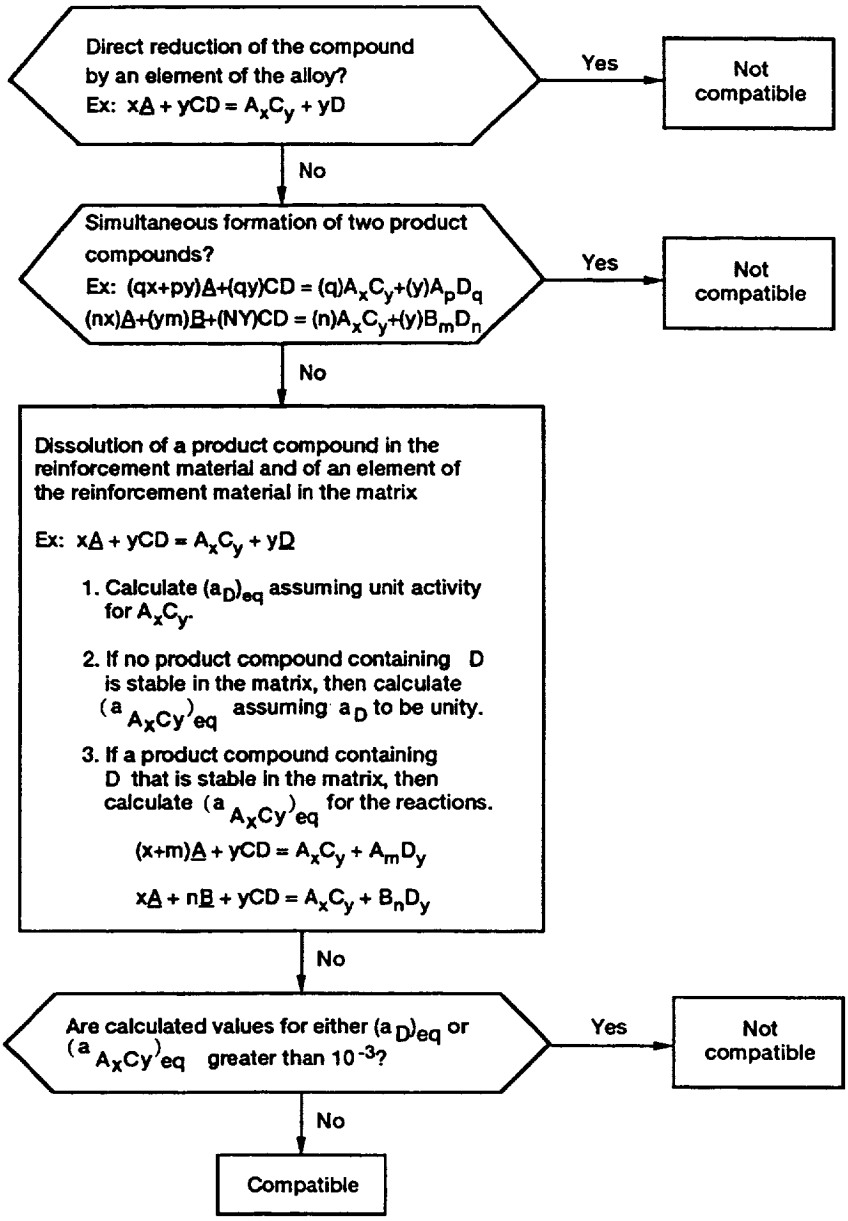

Figure 1. —Sequence of steps in chemical compatibility calculations.

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Chemical compatibility between Fe-19.8Cr-4.8Al (wt. %), which is the base composition for the commercial superalloy MA956, and several carbides, borides, nitrides, oxides, and silicides was analyzed from thermodynamic considerations. The effect of addition of minor alloying elements, such as Ti, Y, and Y_2O_3, to the Fe-Cr-Al alloy on chemical compatibility between the alloy and various compounds was also analyzed. Several chemically compatible compounds that can be potential reinforcement materials and/or interface coating materials for Fe-Cr-Al-based composites were identified.

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