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THERMODYNAMIC ANALYSIS OF CHEMICAL COMPATIBILITY OF SEVERAL REINFORCEMENT MATERIALS WITH NIOBIUM ALUMINIDES

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ABSTRACT

Chemical compatibility of several reinforcement materials with three niobium aluminides, Nb_3Al, Nb_2Al, and $NbAl_3$, were examined from thermodynamic considerations. The reinforcement materials considered in this study include carbides, borides, nitrides, oxides, silicides, and Engel-Brewer compounds. Thermodynamics of the Nb-Al system were reviewed and activities of Nb and Al were derived at desired calculation temperatures. Criteria for chemical compatibility between the reinforcement material and Nb-Al compounds have been defined and several chemically compatible reinforcement materials have been identified.

INTRODUCTION

Fiber-reinforced intermetallic matrix composites are currently being considered as potential high temperature structural materials for future gas turbine engines. The key factors in the selection of a suitable reinforcement material for a given matrix are (1) chemical compatibility of the reinforcement material with the matrix, and (2) a close match in coefficient of thermal expansion (CTE) between the reinforcement material and the matrix. Thermodynamic-based predictions on chemical compatibility of several matrix-reinforcement material combinations can narrow down the choices for composite systems and thus reduce the experimental effort needed to identify potential combinations. In two earlier reports (refs. 1 and 2), chemical compatibility of several reinforcement materials with NiAl and FeAl matrices were analyzed from thermodynamic considerations. The objective of this report is to examine the chemical compatibility of several potential reinforcement materials with niobium aluminides.

Nb-Al SYSTEM

The Nb-Al phase diagram (ref. 3) is shown in figure 1. There are three compounds in the Nb-Al binary system and the melting points plus densities for these three compounds are shown in Table I. The compounds Nb_2Al and Nb_3Al have a limited range of solid solubility on both sides of the stoichiometric composition for the respective compounds, whereas, $NbAl_3$ is a line compound.

The compounds Nb_3Al and Nb_2Al do not appear to have good oxidation resistance (ref. 4) because they fail to form a protective Al_2O_3 scale. However these two compounds, because of their higher melting points, would be attractive for temperatures greater than 1644 K

(2500 F) if these alloys can be made oxidation resistant or if suitable oxidation resistant coatings can be developed for these alloys. $NbAl_3$ would probably be suitable for temperatures lower than 1644 K (2500 F) because of its lower melting point. Since the melting point for $NbAl_3$ is comparable to that of NiAl (1911 K), it is likely that $NbAl_3$ would be suitable at temperatures on the order of 1573 K. Although the oxidation resistance of $NbAl_3$ is inferior to that of NiAl, $NbAl_3$ appears to be attractive because of its lower density ($4.54 gm/cm^3$ as compared to $6 gm/cm^3$ for NiAl).

In this report we will examine the chemical compatibility of all three Nb-Al compounds, i.e. Nb_3Al, Nb_2Al, and $NbAl_3$, with different potential reinforcement materials. Since the compounds Nb_3Al and Nb_2Al are likely to be used above 1644 K, the compatibility of these two compounds will be examined at 1773 K. On the other hand, the compatibility of $NbAl_3$ with different reinforcement materials will be examined at 1573 K.

REVIEW OF THERMODYNAMIC DATA FOR Nb-Al SYSTEM

Thermodynamic calculations on chemical compatibility of intermetallic matrices with reinforcement materials require a knowledge of the activities of the elements in the intermetallic matrix. Shilo et. al. (ref. 5) have measured the vapor pressure of Al in Nb-Al alloys by weight-loss mass spectrometry in the temperature range 1844 - 2146 K and in the composition interval 0-36 a/o Al, which includes both the Nb_3Al and Nb_2Al compounds. The same authors have measured the Al vapor pressure in the two phase region consisting of Nb_2Al and $NbAl_3$ at lower temperatures, i.e. in the temperature range 1379-1785 K. They have used the Al vapor pressure data to calculate the enthalpies of formation of niobium aluminides; however they did not calculate Al and Nb activities in Nb-Al alloys using their own data.

Aluminum vapor pressure data of Shilo et. al in the temperature interval 1844 - 2146 K are shown in figure 2. Utilizing these data, activities of Al in Nb-Al alloys as a function of composition were calculated from the vapor pressure data for pure Al as a function of temperature (ref. 6). Subsquently, Nb activities in the alloy were obtained by Gibbs-Duhem integration of the Al activity data. Utilizing the data shown in figure 2, activities of Al and Nb in both Nb_3Al and Nb_2Al could be calculated only for the temperature range 1844 to 1945 K. At 2146 K, since the maximum Al concentration for which Al vapor pressure measurements were made is only 10 a/o, no calculations were possible for either Nb_3Al or Nb_2Al. Similarly, at 1994 K, the Nb activity could be calculated for the compound Nb_3Al, but not for Nb_2Al.

Niobium and aluminum activities in the $NbAl_3$ phase would be the same as that in Nb_2Al solid solution for Al concentrations corresponding to the $Nb_2Al/NbAl_3$ phase boundary. Unfortunately, Al vapor pressure data shown in figure 2 does not extend to Al concentrations corresponding to the $Nb_2Al/NbAl_3$ phase boundary. However, Al vapor pressure measrements have been made in the two phase region consisting of Nb_2Al and $NbAl_3$ within the temperature range 1379 -1785 K. These data, if extrapolated to higher temperatures and then combined with the vapor pressure data for the Nb_2Al solid solution, can be used to calculate Nb and Al activity in $NbAl_3$ since Al vapor pressure in this two phase region would be the same as that in the Nb_2Al phase at $Nb_2Al/NbAl_3$ phase boundary. Shilo et. al. have obtained a least squares expression for the vapor pressure of Al in the Nb_2Al plus $NbAl_3$ two phase region as a function of temperature in the range 1379 - 1785 K. This expression was extrapolated to higher temperatures in order to obtain Nb and Al activities in $NbAl_3$ phase.

The calculated niobium and aluminum activities in Nb_3Al, Nb_2Al, and $NbAl_3$ phases at 1844 K are shown in Table II. Since thermochemical compatibility calculations for Nb aluminides will be performed at temperatures lower than 1844 K, the activity data shown in Table II need to be extrapolated to lower temperatures. This can be done via the expression

$$RT_1 \ln\tau_1 = RT_2 \ln\tau_2 \qquad [1]$$

where T_1 and T_2 are two different temperatures; τ_1 and τ_2 are the activity coefficients at temperatures T_1 and T_2, respectively. Table III gives the calculated activities of Nb and Al in Nb aluminides at the temperatures of interest.

REINFORCEMENT MATERIALS CONSIDERED

Reinforcement materials considered in this study, shown in Table IV, include carbides, borides, oxides, nitrides, silicides, and a few Engel-Brewer type compounds.

CALCULATION PROCEDURES

The reactions between the intermetallic matrix and the reinforcement material can be grouped under three categories, which are:

(1) Reduction of the reinforcement material by an element of the intermetallic matrix.

(2) Simultaneous formation of two product compounds.

(3) Dissolution of elements of the reinforcement material in the matrix and of the matrix in the reinforcement material.

Each of these modes of reaction will be discussed below in detail with suitable examples. The sequence of steps necessary to determine the compatibility of a given reinforcement material with the matrix are outlined in figure 3. The matrix and reinforcement material are represented as AB and CD, respectively. The underline in a given reaction denotes that the element or the compound is present at a reduced activity. No ternary or higher order compounds are considered in the calculations because of a lack of thermodynamic data for Nb-Al-X-Y (X, Y are other elemnets) type compounds.

Reduction of the reinforcement material by an element of the intermetallic matrix: As an example, consider the reaction of $NbAl_3$ with SiC. The stable carbide compound in a $NbAl_3$ matrix would be NbC (assuming no ternary compounds). The reduction reaction in which NbC is formed and SiC is reduced to free Si can be writtn as:

$$\underline{Nb} + SiC = NbC + Si \qquad [2]$$

The activities of SiC and NbC are unity and, for formation of free Si, the activity of Si would also be unity. Thus the equilibrium constant for reaction [2] can be written as

$$K_2 = 1/(a_{Nb}) \qquad [3]$$

where K_2 is the equilibrium constant for reaction 2 (in subsquent reactions, K_i would be the equilibrium constant for reaction [1]) and a_{Nb} is the activity of Nb in the alloy. If the activity of Nb in the alloy is greater than that calculated from eqn. [3], i.e. the equilibrium (a_{Nb}) value for reaction [3], then reaction [2] would proceed in the forward direction and the reinforcement material would be reduced by Nb. The equilibrium a_{Nb} value for reaction [2] at 1573 K is calculated to be $1.787*10^{-3}$, while the activity of Nb in $NbAl_3$ at 1573 K is 0.237.at 1573 K. Therefore SiC will be reduced by the Nb component of the alloy resulting in formation of NbC and free Si. Thus $NbAl_3$ would not be chemically compatible with SiC.

The first step in chemical compatibility calculations is to examine if a reduction reaction similar to that of reaction [2] is feasible. If this is the case, then the reinforcement material would not be compatible with the matrix and further calculations are not necessary.

Simultaneous formation of two product compounds: If a direct reduction reaction similar to that of reaction [2] is not feasible, the next step is to examine if two product compounds can be formed simultaneously as a result of the reaction of the intermetallic matrix with the reinforcement material. There can be two scenarios: (a) one component of the intermetallic matrix reacting with the reinforcement material to form two product compounds simultaneously or (b) both components of the intermetallic matrix reacting with the reinforcement material to form two product compounds simultaneously.

As an example of the first scenario in which one component of the intermetallic matrix can react with the reinforcement material to form two product compounds simultaneously, let us consider the reaction of $NbAl_3$ with CeO_2. The stable oxide for a $NbAl_3$ matrix is Al_2O_3. Thus, as described in the previous section, the first step will be to examine if CeO_2 can be reduced by the Al component of the alloy to form Al_2O_3 and free Si via the reaction:

$$4\underline{Al} + 3CeO_2 = 2Al_2O_3 + 3Ce \qquad [4]$$

From equilibria considerations for the above reaction at 1573 K, it is determined that the Al activity in the alloy must be greater than 0.397 for reduction of CeO_2 to form Al_2O_3 and pure Ce. Since the Nb activity in $NbAl_3$ is less than this, reaction [4] is not feasible. Although free Ce (Ce at unit activity) cannot be formed by reaction [4], Ce can be formed at a reduced activity, i.e. Ce will be dissolved in the matrix. The dissolved Ce can combine with Al to form Al_2Ce and this will lead to formation of two compounds, Al_2O_3 and Al_2Ce, simultaneously by reaction of the Al component of the alloy with CeO_2. Now let us examine the conditions necessary for the formation of these two compounds simultaneously. The reaction can be written as

$$10\underline{Al} + 3CeO_2 = 2Al_2O_3 + 3Al_2Ce \qquad [5]$$

and, assuming activities of CeO_2, Al_2O_3, and Al_2Ce to be unity, the equilibrium constant for reaction [5] can be expreseed as:

$$K_5 = 1/(a_{Al})^{10} \qquad [6]$$

Thus if a_{Al} in the alloy is greater than $(1/K_5)^{0.1}$, the compounds Al_2O_3 and Al_2Ce can be formed simultaneously. The calculated equilibrium a_{Al} for reaction [5] at 1573 K is 0.027. The activity of Al in $NbAl_3$ at 1573 K (0.0496) is greater than this; therefore reaction of $NbAl_3$ with CeO_2 will lead to formation of Al_2O_3 and Al_2Ce simultaneously. Thus, even if free Ce is not generated as a result of direct reduction of CeO_2, $NbAl_3$ would not be compatible with CeO_2 because of simultaneous formation of Al_2O_3 and Al_2Ce.

Now, let us consider the second scenario in which both the elements of the reinforcement material can react with the reinforcement material to form two product compounds simultaneously. Consider, as an example, reaction of $NbAl_3$ with BN. First consider the direct reduction of BN by the Al component of the matrix to form AlN and free B via the reaction:

$$\underline{Al} + BN = AlN + B \qquad [7]$$

In order for AlN and free boron to be formed by the above reaction at 1573 K, the Al activity in the alloy must be greater than 0.059. Since the Al activity in $NbAl_3$ is 0.049, which is less than that required for formation of AlN and free B, straightforward reduction of BN by Al component of the alloy is not possible. However boron can be generated at a reduced activity, i.e. it can be dissolved in the matrix, and dissolved B can combine with the Nb component of the alloy resulting in precipitation of NbB_2. These reactions can be written as:

$$\underline{Al} + BN = AlN + \underline{B} \qquad [8]$$
$$\underline{Nb} + 2\underline{B} = NbB_2 \qquad [9]$$

Combining reactions [8] and [9] we obtain

$$2\underline{Al} + \underline{Nb} + 2BN = 2AlN + NbB_2 \qquad [10]$$

for which, assuming unit activity for BN, AlN, and NbB_2, the equilibrium constant can be expressed as

$$K_{10} = 1/\{(a_{Al})^2*(a_{Nb})\} \qquad [11]$$

and, if the product $(a_{Al})^2*(a_{Nb})$ in the alloy is greater than $1/K_{10}$, simultaneous formation of AlN and NbB_2 would be possible. Thus, for reaction [10] to occur at 1573 K, the product $(a_{Al})^2*(a_{Nb})$ in the alloy must be greater than $4.143*10^{-8}$. From the activity data in Table III, the product $(a_{Al})^2*(a_{Nb})$ in $NbAl_3$ is $5.83*10^{-4}$ which is much higher than that required for simultaneous formation of AlN and NbB_2. Thus, even if the activity of Al is not sufficient to form AlN and free boron by reaction [8], AlN and NbB_2 can be formed simultaneously by reaction of both Nb and Al with BN. This would clearly make BN incompatible with $NbAl_3$.

Dissolution of elements of the matrix in the reinforcement material and of elements of the reinforcement materials in the matrix:

In the absence of any compound formation, dissolution of the elements of the reinforcement material in the matrix and of the elements of the matrix in the reinforcement material would be the predominant mode of reaction.

As an example, let us consider reaction of $NbAl_3$ with HfC. The stable C-containing compound that can form in the matrix is NbC. Similarly the stable Hf-containing compound that can form in the matrix is Al_2Hf. Examination of the equilibria for the reactions

$$\underline{Nb} + HfC = NbC + Hf \qquad [12]$$

$$2\underline{Al} + HfC = Al_2Hf + C \qquad [13]$$

shows that direct reduction of HfC by either Nb or Al component of the alloy is not feasible. Also, the product $(a_{Nb})*(a_{Al})^2$ in the alloy is less than that required for simultaneous formation of Al_2Hf and NbC via the reaction:

$$\underline{Nb} + 2\underline{Al} + HfC = NbC + Al_2Hf \qquad [14]$$

Since direct reduction and simultaneous formation of two product compounds are not feasible, reaction between $NbAl_3$ and HfC will occur by (1) dissolution of Hf and C in the matrix, and (2) dissolution of Nb and Al in the reinforcement material.

Although NbC and free Hf (Hf at unit activity) are not formed as a result of reaction [12], Hf can still be formed at a reduced activity, i.e. Hf will be dissolved in the matrix instead of being formed at unit activity. Thus reaction [12] can be rewritten as

$$\underline{Nb} + HfC = NbC + \underline{Hf} \qquad [15]$$

and the equilibrium constant for this reaction is:

$$K_{15} = a_{Hf}/a_{Nb} \qquad [16]$$

The Nb component of the alloy will continue to react with HfC resulting in formation of NbC and dissolution of Hf in the matrix until the activity of Hf in the matrix becomes equal to $K_{15}*a_{Nb}$, which may be designated as $(a_{Hf})_{eq}$. Similarly, even if Al_2Hf and pure carbon (carbon at unit activity) cannot be formed by reaction [13], carbon can be formed at a reduced activity, i.e. because of being dissolved in the matrix by the reaction

$$2\underline{Al} + HfC = Al_2Hf + \underline{C} \qquad [17]$$

for which the equilibrium constant is:

$$K_{17} = a_C/(a_{Al})^2 \qquad [18]$$

Reaction [17] will continue to proceed in the forward direction until the carbon activity in the matrix becomes equal to $K_{17}*(a_{Al})^2$, which may be designated as $(a_C)_{eq}$. The higher the values for $(a_{Hf})_{eq}$ and $(a_C)_{eq}$ are, the greater will be the extent of reaction between the reinforcement material and the matrix. Therefore lower numbers for $(a_C)_{eq}$ and $(a_{Hf})_{eq}$ are desired for the reinforcement material to be compatible with the matrix. In the present calculations, if the values of $(a_C)_{eq}$ and $(a_{Hf})_{eq}$ are less than 10^{-3}, the reinforcement material is considered to be compatible with the matrix. For $NbAl_3$-HfC combination at 1573 K, $(a_{Hf})_{eq}$ and $(a_C)_{eq}$ are calculated to be $4.6*10^{-4}$ and $6.376*10^{-5}$, respectively, and therefore, HfC can be considered to be compatible with $NbAl_3$. However, so far, we have not considered dissolution of elements of the matrix in the reinforcement material and this will be discussed in the next paragraph.

Hafnium carbide can dissolve large amounts of Nb since HfC and NbC are known to form a continuous series of solid solution (ref. 7). In reaction [15], only formtion of Hf at a reduced activity was considered. Now let us consider formation of both NbC and Hf at reduced activities, which is equivalent to dissolution of NbC in HfC and dissolution of Hf in the matrix. Then Nb component of the matrix will continue to react with HfC via

$$\underline{Nb} + HfC = \underline{NbC} + \underline{Hf} \qquad [19]$$

for which the equilibrium constant can be written as:

$$K_{19} = (a_{NbC})*(a_{Hf})/a_{Nb} \qquad [20]$$

Reaction [19] will proceed in the forward direction until the product $(a_{NbC})*(a_{Hf})$ becomes equal to $K_{19}*(a_{Nb})$. For the $NbAl_3$-HfC combination at 1573 K the product of activities is calculated to be $4.6*10^{-4}$. Thus if it is assumed that Hf is formed at unit activity, then $(a_{NbC})_{eq}$ will be $4.6*10^{-4}$. However, any decrease in the activity of Hf in the system will increase the activity of NbC in HfC and will lead to increased dissolution of NbC in HfC. The activity of Hf can clearly be reduced via formation of Al_2Hf by the reaction:

$$2\underline{Al} + \underline{Hf} = Al_2Hf \qquad [21]$$

Combination of reactions [19] and [21] leads to

$$\underline{Nb} + 2\underline{Al} + HfC = \underline{NbC} + Al_2Hf \qquad [22]$$

and the equilibrium constant for this reaction is:

$$K_{22} = a_{NbC}/\{(a_{Nb})*(a_{Al})^2\} \qquad [23]$$

Reaction [22] is the same as reaction [14] with one added feature, i.e., NbC is now dissolved in HfC instead of being formed at unit activity. Both Nb and Al components of the alloy will continue to react with HfC leading to formation of Al_2Hf and dissolution of NbC in HfC until the activity of NbC in HfC equals $K_{18}*a_{Nb}*(_{Al})^2$, which can be designated as $(a_{NbC})_{eq}$. For the $NbAl_3$-HfC combination at 1573 K, $(a_{NbC})_{eq}$ for reaction [22] is 0.213, which is fairly large. Thus reaction of $NbAl_3$ with HfC will lead to formation of Al_2Hf along with dissolution of a considerable amount of NbC in HfC and this renders HfC incompatible with $NbAl_3$.

In general, if the calculated values of either the equilibrium activities for elements of the reinforcement material in the matrix or of the product compounds in the reinforcement material are less than 10^{-3}, the reinforcement material will be considered to be compatible with the matrix. It must be noted that the number 10^{-3} is an arbitrary one and is primarily for screening purposes only. In many instances, if the calculated equilibrium activity values are greater than 10^{-3}, the reinforcement material may still be considered to be compatible with the matrix provided the solubilities of the elements of the reinforcement material in the matrix and of the product compound in the reinforcement material are negligible.

IDENTIFICATION OF STABLE PRODUCT COMPOUNDS

As evident from the above discussions, compatibility calculations require writing of suitable reactions in which an element of the intermetallic matrix reacts with the reinforcement material to form a product compound. Determination of a product compound in a given reaction requires three steps and these will be demonstrated below with an example of reaction of Nb-Al compounds with the carbon component of the carbides.

(1) The first step is to identify possible binary product compounds. In the case of a reaction of Nb-Al alloy with carbide reinforcement materials, binary Nb-C and Al-C compoundsneed to beconsidered. It should be noted that ternary or higher order compounds are not considered in the present calculations. There are two compounds in the Nb-C system: Nb_2C and NbC. Of these two compounds NbC is the most stable compound and this will be considered in the calculations. In the binary system Al-C, Al_4C_3 is the most stable compound.

(2) The next step is to determine if minimum conditions are satisfied for the formation of these binary compounds. Formation of NbC

requires that the activity product $(a_{Nb})*(a_C)$ must be greater than the equilibrium constant for the reaction

$$\underline{Nb} + \underline{C} = NbC \qquad [24]$$

which is:

$$K_{24} = 1/\{(a_{Nb})*(a_C)\} \qquad [25]$$

Assuming carbon activity to be unity, the equilibrium activity of Nb for reaction [24] becomes equal to K_{24}. Thus, if the Nb activity in the alloy is less than K_{24}, NbC cannot be formed even if the carbon activity is unity, i.e., even if the alloy is in contact with pure carbon. Similarly, minimum conditions for the formation of Al_4C_3 would be satisfied if the Al activity in the alloy must be greater than $(K_{26})^{1/4}$, where K_{26} is the equilibrium constant for the reaction

$$4\underline{Al} + 3\underline{C} = Al_4C_3 \qquad [26]$$

For the Nb-Al compounds, $NbAl_3$, Nb_2Al, and Nb_3Al, calculations show that the minimum conditions are satisfied for formation of both NbC and Al_4C_3.

(3) Since the minimum conditions are satisfied for the formation of both NbC and Al_4C_3, the next step is to determine the relative stabilities of these two carbides in a Nb-Al matrix which is governed by the equilibria for the reaction

$$3\underline{Nb} + Al_4C_3 = 3NbC + 4\underline{Al} \qquad [27]$$

for which the equilibrium constant is expressed as:

$$K_{27} = (a_{Al})^4/(a_{Nb})^3 \qquad [28]$$

Thus, if the activity ratio $(a_{Al})^4/(a_{Nb})^3$ in the alloy is less than K_{27}, NbC would be the stable carbide in the Nb-Al matrix; otherwise Al_4C_3 would be the stable carbide in the matrix. For all the Nb-Al compounds considered in the present calculations, NbC is the stable carbide in the matrix and will be considered as the product compound for reaction of Nb-Al alloys with carbides.

Table V gives the stable product compounds in the matrix for different elements of the reinforcement materials.

RESULTS OF CALCULATIONS

Thermodynamic data for different compounds are given in Appendix A.

Compatibility with carbides: Results of the thermodynamic calculations for carbide reinforcement materials are given in detail in Tables VI and VII. Only NbC appears to be compatible with any of the Nb-Al compounds.

Compatibility with borides: Results of the thermodynamic calculations for boride reinforcement materials are given in detail in Tables VIII and IX. The stable product compound for reaction of all three Nb-Al compounds with the boron component of the boride reinforcement materials is NbB_2. Besides NbB_2, the borides that are compatible in all three Nb-Al compounds are ScB_2, TiB_2, HfB_2, and NbB_2. The compound ZrB_2 is compatible with Nb_3Al and Nb_2Al, but iis compatibility with $NbAl_3$ is marginal since the equilibrium NbB_2 activity for the reaction

$$\underline{Nb} + 2\underline{Al} + ZrB_2 = \underline{NbB}_2 + Al_2Zr \qquad [29]$$

is calculated to be $4.72*10^{-3}$ at 1573 K. However, if ZrB_2 is doped with a small amount of NbB_2 such that activity of NbB_2 is equal to $4.72*10^{-3}$, reaction [29] cannot proceed in the forward direction and ZrB_2 can be compatible with $NbAl_3$.

Compatibility with oxides: Results of thermodynamic calculations for compatibility of the Nb-Al compounds with oxide reinforcement materials are given in Table X and XI. The oxide reinforcement materials that are compatible with all three Nb-Al compounds are: Al_2O_3, BeO, Gd_2O_3, HfO_2, La_2O_3, Sc_2O_3, and Y_2O_3. The oxides CaO and ZrO_2 appear to be compatible with Nb_3Al and Nb_2Al, but not with $NbAl_3$.

The oxide MgO would be compatible with all three Nb-Al compounds if the matrix-reinforcement material is not exposed to a dynamic gaseous envionment. The equilibrium partial pressure of Mg for the reaction

$$2\underline{Al} + 3MgO = Al_2O_3 + 3Mg(g) \qquad [30]$$

is calculated to be 0.032 atm. for the $NbAl_3$-MgO interface at 1573 K, 0.063 atm. for Nb_2Al-MgO interface at 1773 K, and 0.057 atm. for the Nb_3Al-MgO interface at 1573 K. These equilibrium partial pressures of Mg are relatively high and,in a dynamic environment in which the product gases are continuously swept away, reaction [30] will proceed in the forward direction resulting in conversion of MgO to Al_2O_3. However, in a closed system where the reinforcement material is completely sealed inside the matrix, Mg is formed at a reduced activity by being dissolved in the alloy and the equilibrium Mg activity for the reaction

$$2\underline{Al} + 3MgO = Al_2O_3 + 3\underline{Mg} \qquad [31]$$

is on the order of 10^{-4} for Nb_3Al and Nb_2Al, and on the order of 10^{-3} for $NbAl_3$. Thus MgO would be compatible with all three Nb-Al compounds in a closed system.

Compatibility with nitrides: Results of thermodynamic calculations for nitride reinforcement materials are shown in detail in Tables XII and XIII. The stable product nitride compound for reaction of Nb_2Al and Nb_3Al with nitride reinforcement materials is Nb_2N. This is the only nitride found to be compatible with Nb_2Al and Nb_3Al. The compatibility of three other nitrides, HfN, ZrN, and TiN are marginal, and can be considered to be compatible if a small amount of reaction can be tolerated. Also, these three reinforcement materials can be made to be compatible with the matrices with small modifications to either reinforcement material or matrix compositions. For example, ZrN can be made to be compatible with Nb_3Al and Nb_2Al if a small amount of Nb is added to ZrN such that the activity of Nb_2N in the reinforcement material becomes equal to the equilibrium Nb_2N activity for the reaction:

$$2\underline{Nb} + 2\underline{Al} + ZrN = \underline{Nb_2N} + Al_2Zr \qquad [32]$$

This is calculated to be $8.13*10^{-3}$ and $8.35*10^{-3}$ for Nb_2Al and Nb_3Al, respectively. The primary mode of reaction for TiN is the formation of Nb_2N and dissolution of Ti in matrix. This reinforcement material could be made compatible with Nb_3Al and Nb_2Al if a small amount of Ti is dissolved in the matrix such that the activity of Ti in the matrix becomes equal to to the equilibrium Ti activity for the reaction:

$$2\underline{Nb} + TiN = Nb_2N + \underline{Ti} \qquad [33]$$

The stable product nitride compound for reaction of $NbAl_3$ with nitride reinforcement materials is AlN. This is the only nitride compatible with $NbAl_3$. TiN appears to be marginally compatible, however its compatibility with $NbAl_3$ can be improved by adding a small amount of AlN to it such that the activity of AlN in TiN becomes equal to $4.64*10^{-3}$ which is the equilibrium AlN activity for the reaction:

$$2\underline{Al} + TiN = TiAl + \underline{AlN} \qquad [34]$$

Compatibility with silicides: Results of thermodynamic calculations for compatibility of Nb-Al compounds with silicide reinforcement materials are given in Table XIV. Nb_5Si_3 appears to be the only stable silicide in all three Nb-Al compounds.

Compatibility with Engel-Brewer compounds: Table XV gives the results of thermodynamic calculations for compatibility of Nb-Al compounds with different Engel-Brewer compounds. None of these intermetallic compounds are compatible with $NbAl_3$. Only one Engel-Brewer compound, PtHf, might be compatible with Nb_3Al and Nb_2Al.

LIST OF COMPATIBLE REINFORCEMENT MATERIALS

Reinforcement materials compatible with Nb_3Al and Nb_2Al: The reinforcement materials that are compatible with Nb_3Al and Nb_2Al are:

NbC, ScB_2, TiB_2, HfB_2, ZrB_2, Al_2O_3, BeO, CaO, Gd_2O_3, HfO_2, La_2O_3, Sc_2O_3, Y_2O_3, ZrO_2, and Nb_5Si_3

Besides these, HfN, TiN, ZrN, and PtHf are marginally compatible and the compatibility of these reinforcement materials can be improved by making small modifications to the matrix and reinforcement material compositions. Also, MgO would be compatible with Nb_3Al and Nb_2Al if the reinforcement material is completely embedded in the matrix.

Since ZrO_2, Y_2O_3, and CaO are all stable in Nb_3Al and Nb_2Al, calcia and yttria stabilized ZrO_2 would also be compatible with these two Nb-Al compounds.

Reinforcement materials compatible with $NbAl_3$: The reinforcement materials that are compatible with $NbAl_3$ are:

NbC, NbB_2, ScB_2, TiB_2, AlN, Al_2O_3, BeO, Gd_2O_3, HfO_2, La_2O_3, Sc_2O_3, Y_2O_3, and Nb_5Si_3.

The compatibility of two borides, HfB_2 and ZrB_2, are marginal and could be compatible with $NbAl_3$ if they were doped with a small amount of NbB_2. Similarly, the reinforcement material TiN, whose compatibility with $NbAl_3$ appears to be marginal, can be made to be compatible with $NbAl_3$ by adding a small amount of AlN. Magnesium oxide would be compatible with $NbAl_3$ if the oxide is completely sealed inside the matrix.

SUMMARY AND CONCLUDING REMARKS

Thermodynamic calculations have been performed to identify potential reinforcement materials that are chemically compatible with different Nb-Al compounds and several candidate reinforcement materials have been identified. One of the prime limitations of the present study is that ternary compounds were not considered because of lack of thermodynamic data for higher order compounds. It is possible that some of the reinforcement materials that are classified as compatible may not be so if ternary compounds are considered. However this does not defeat the basic purpose of this study which is to screen several potential reinforcement materials so that the choices can be narrowed down to only a few. Clearly, we have achieved this objective by identifying only 15-20 potential reinforcement materials from a list of about seventy. These candidate materials will undergo detailed experimental studies.

In addition to chemical compatibility between the reinforcement material and the matrix, the coefficient of thermal exapansion (CTE) of the reinforcement material must match closely with that of the matrix in order to avoid large thermal stresses during cooling. There are no measured values in the open literature for thermal expansion of Nb-Al compounds. Recent measurements by Hebsur (ref. 8) for the thermal expansion of a $NbAl_3$-based alloy containing Cr, Y, and Si yields a CTE of $10*10^{-6}$ K^{-1} at 1473 K. Thus many of the chemically compatible reinforcement materials, i.e. Al_2O_3, BeO, Sc_2O_3, TiB_2, and Y_2O_3, would have a close match in CTE with $NbAl_3$. This would make $NbAl_3$-based composite systems very promising as compared to NiAl and FeAl-based composite systems in which, because of larger expansion coefficients for these two aluminides ($\tilde{}16*10^{-6}$ K^{-1} for NiAl and $\tilde{}21*10^{-6}$ K^{-1} for FeAl), it is difficult to find a suitable reinforcement material with a close match in CTE with that of the matrix (refs. 1 and 2).

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Table I
Melting points and densities for Nb-Al compounds

Compound	Melting Point (K)	Density (gm/cm^3)
Nb_3Al	2233	7.29
Nb_2Al	2143	6.87
$NbAl_3$	1878	4.54

TABLE II
Nb and Al activities in niobium alumimides at 1844 K
(activity of Nb is with respect to b.c.c. Nb)
(activity of Al is with respect to liquid Al)

Aluminide Phase	Activity of Nb (a_{Nb})	Activity of Al (a_{Al})
Nb_3Al	0.726	0.0148
Nb_2Al	0.544	0.0174
$NbAl_3$	0.239	0.0739

TABLE III
Activities of Nb and Al in Nb aluminides at temperatures of interest in this study
(Nb activity is with respect to b.c.c.Nb)
(Al activity is with respect to liquid Al)

Aluminide	Temperature (K)	a_{Nb}	a_{Al}
Nb_3Al	1773	0.725	0.0132
Nb_2Al	1773	0.54	0.0155
$NbAl_3$	1573	0.237	0.0496

TABLE IV
Reinforcement materials considered in this study

Carbides	Borides	Oxides	Nitrides	Silicides	Engel-Brewer compounds
B_4C	AlB_{12}	Al_2O_3	AlN	Cr_3Si	HfPt
HfC	CrB_2	BeO	BN	Cr_5Si_3	$HfPt_3$
Mo_2C	HfB_2	CaO	HfN	Mo_3Si	$NbCr_2$
NbC	LaB_6	CeO_2	LaN	Mo_5Si_3	TiIr
SiC	NbB_2	Cr_2O_3	Si_3N_4	$MoSi_2$	$TiIr_3$
TaC	ScB_2	Gd_2O_3	TaN	Nb_5Si_3	TiPt
Ta_2C	TaB_2	HfO_2	TiN	$NbSi_2$	$TiPt_3$
TiC	TiB_2	La_2O_3	ZrN	Ta_2Si	$ZrIr_3$
V_2C	TiB	MgO		Ta_5Si_3	ZrPt
VC	VB	Sc_2O_3		$TaSi_2$	$ZrPt_3$
W_2C	VB_2	SiO_2		Ti_5Si_3	
WC	V_3B_2	TiO		TiSi	
ZrC	V_2B_3	TiO_2		V_3Si	
	ZrB_2	Y_2O_3		V_5Si_3	
		ZrO_2		VSi_2	
				W_5Si_3	
				WSi_2	
				Zr_2Si	
				Zr_5Si_3	
				ZrSi	

TABLE V

Product compounds considered for different elements

Element	Stable Product compound in the matrix
B	NbB_2
Be	- No product compound considered-
C	NbC
Ca	$CaAl_2$
Ce	$CeAl_2$
Cr	Cr_4Al_6 for $NbAl_3$; No product compound for Nb_3Al and Nb_2Al
Gd	- No product compound considered-
Hf	Al_2Hf
Ir	AlIr
La	$LaAl_2$ for $NbAl_3$; no product compounds for Nb_3Al and Nb_2Al
Mg	- No product compound considered-
Mo	- No product compound considered-
N	AlN for $NbAl_3$; Nb_2N for Nb_3Al and Nb_2Al.
O	Al_2O_3
Pt	AlPt
Sc	- No product compound considered-
Si	Nb_5Si_3
Ta	- No product compound considered-
Ti	TiAl for $NbAl_3$; No product compound for Nb_3Al and Nb_2Al
V	- No product compound considered-
W	- No product compound considered-
Y	- No product compound considered-
Zr	Al_2Zr

TABLE VI

Compatibility of Nb_3Al and Nb_2Al with carbides at 1773 K

Carbide	Mode of reaction	Comments on compatibility
B_4C	1. Formation of NbC and free boron: $\underline{Nb} + B_4C = NbC + 4B$ 2. Formation of NbB_2 and free carbon: $2\underline{Nb} + B_4C = 2NbB_2 + C$	Not compatible
HfC	Formation of Al_2Hf and dissolution of NbC in HfC Reaction: $\underline{Nb} + 2\underline{Al} + HfC = \underline{NbC} + Al_2Hf$ $(a_{NbC})_{eq} = 0.024$ for Nb_3Al $= 0.025$ for Nb_2Al	Not compatible
Mo_2C	Formation of NbC and free Mo $\underline{Nb} + Mo_2C = NbC + 2Mo$	Not compatible
NbC	Stable in the matrix	Compatible
SiC	1. Formation of NbC and free Si $\underline{Nb} + SiC = NbC + Si$ 2. Formation of Nb_5Si_3 and free C $5\underline{Nb} + 3SiC = Nb_5Si_3 + 3C$	Not compatible
TaC	Dissolution of Ta in matrix and of Nb in TaC: Reaction: $\underline{Nb} + TaC = \underline{NbC} + \underline{Ta}$ $(a_{Ta})*(a_{NbC}) = 0.52$ for Nb_3Al $= 0.39$ for Nb_2Al	Not compatible

TABLE VI (contd.)
Compatibility of Nb_3Al and Nb_2Al with carbides at 1773 K

Carbides	Mode of reaction	Comments on compatibility
Ta_2C	Formation of NbC and dissolution of Ta in matrix Reaction: $\underline{Nb} + Ta_2C = NbC + 2\underline{Ta}$ $(a_{Ta})_{eq} = 0.104$ for Nb_3Al $= 0.091$ for Nb_2Al	Not compatible
TiC	Dissolution of Nb in TiC and of Ti in matrix: Reaction: $\underline{Nb} + TiC = \underline{NbC} + \underline{Ti}$ $(a_{NbC})*(a_{Ti}) = 0.129$ for Nb_3Al $= 0.09$ for Nb_2Al	Not compatible
VC	Formation of NbC and free V Reaction: $\underline{Nb} + VC = NbC + V$	Not compatible
V_2C	Dissolution of V in matrix and of Nb in V_2C: Reaction: $\underline{Nb} + V_2C = \underline{NbC} + 2\underline{V}$ $(a_{NbC})*(a_V)^2 = 0.611$ for Nb_3Al $= 0.129$ for Nb_2Al	Not compatible
WC	Formation of NbC and free W Reaction: $\underline{Nb} + WC = NbC + W$	Not compatible
W_2C	Formation of NbC and free W Reaction: $\underline{Nb} + W_2C = NbC + 2W$	Not compatible
ZrC	Formation of Al_2Zr and dissolution of NbC in ZrC: Reaction: $\underline{Nb}+2\underline{Al}+ZrC = \underline{NbC}+Al_2Zr$ $(a_{NbC})_{eq} = 0.735$ for Nb_3Al $= 0.755$ for Nb_2Al	Not compatible

TABLE VII
Compatibility of $NbAl_3$ with carbides at 1573 K

Carbide	Mode of reaction	Comments on compatibility
B_4C	Formation of NbC and free B Reaction: $\underline{Nb} + B_4C = NbC + 4B$ Formation of NbB_2 and free C Reaction: $2\underline{Nb} + B_4C = 2NbB_2 + C$	Not compatible
HfC	Formation of Al_2Hf and dissolution of NbC in HfC: Reaction: $\underline{Nb}+2\underline{Al}+HfC = \underline{NbC} + Al_2Hf$ $(a_{NbC})_{eq} = 0.213$	Not compatible
Mo_2C	Formation of NbC and free Mo Reaction: $\underline{Nb} + Mo_2C = NbC + 2Mo$	Not compatible
NbC	Stable in the matrix	Compatible
SiC	Formation of NbC and free Si Reaction: $\underline{Nb} + SiC = NbC + Si$ Formation of Nb_5Si_3 and free C Reaction: $5\underline{Nb}+3SiC =Nb_5Si_3+3C$	Not compatible
TaC	Dissolution of Nb in TaC and of Ta in the matrix: Reaction: $\underline{Nb} + TaC = \underline{NbC} + \underline{Ta}$ $(a_{NbC})*(a_{Ta}) = 0.17$	Not compatible
Ta_2C	Formation of NbC and dissolution of Ta in the matrix: Reaction: $\underline{Nb} + Ta_2C = NbC + 2\underline{Ta}$ $(a_{Ta})_{eq} = 0.094$	Not compatible

TABLE VII (contd.)

Compatibility of $NbAl_3$ with carbides at 1573 K

Carbide	Mode of reaction	Comments on compatibility
TiC	Formation of TiAl and dissolution of NbC in TiC: Reaction: $\underline{Nb}+\underline{Al}+TiC = TiAl+\underline{NbC}$ $(a_{NbC})_{eq} = 0.082$	Not compatible
VC	Formation of NbC and free V Reaction: $\underline{Nb} + VC = NbC + V$	Not compatible
V_2C	Dissolution of Nb in V_2C and of V in the matrix: Reaction: $\underline{Nb} + V_2C = \underline{NbC} + 2\underline{V}$ $(a_{NbC})*(a_V)^2 = 0.147$	Not compatible
WC	Formation of NbC and free W Reaction: $\underline{Nb} + WC = NbC + W$	Not compatible
W_2C	Formation of NbC and free W Reaction: $\underline{Nb} + W_2C = NbC + 2W$	Not compatible
ZrC	Formation of NbC and Al_2Zr Reaction: $\underline{Nb}+2\underline{Al}+ZrC = NbC+Al_2Zr$	Not compatible

TABLE VIII
Compatibility of Nb_3Al and Nb_2Al with borides at 1773 K

Boride	Mode of reaction	Comments on compatibility
AlB_{12}	NbB_2 stable in matrix -- formation of NbB_2.	Not compatible
CrB_2	Formation of NbB_2 and free Cr Reaction: $\underline{Nb} + CrB_2 = NbB_2 + Cr$	Not compatible
HfB_2	Formation of Al_2Hf and dissolution of NbB_2 in HfB_2: Reaction: $\underline{Nb}+2\underline{Al}+HfB_2 = Al_2Hf+\underline{NbB_2}$ $(a_{NbB2})_{eq} = 1.42*10^{-4}$ for Nb_3Al $= 1.45*10^{-4}$ for Nb_2Al	Compatible
LaB_6	Formation of NbB_2 and free La Reaction: $3\underline{Nb} + LaB_6 = 3NbB_2 + La$	Not compatible
NbB_2	NbB_2 stable in the matrix	Compatible
ScB_2	Dissolution of Sc in matrix and of NbB_2 in ScB_2. Reaction: $\underline{Nb} + ScB_2 = \underline{NbB_2} + \underline{Sc}$ $(a_{NbB2})*(a_{Sc}) = 3.2*10^{-5}$ for Nb_3Al $= 2.38*10^{-5}$ for Nb_2Al	Compatible
TaB_2	Dissolution of Ta in matrix and of NbB_2 in TaB_2: Reaction: $\underline{Nb} + TaB_2 = \underline{NbB_2} + \underline{Ta}$ $(a_{NbB2})*(a_{Ta}) = 0.077$ for Nb_3Al $= 0.057$ for Nb_2Al	Not compatible

TABLE VIII (contd.)
Compatibility of Nb_3Al and Nb_2Al with borides at 1773 K

Boride	Mode of reaction	Comments on compatibility
TiB_2	Dissolution of Ti in matrix and of NbB_2 in TiB_2: Reaction: $\underline{Nb} + TiB_2 = \underline{NbB_2} + \underline{Ti}$	
	(1)Barin and Knacke data for H_{298} of TiB_2: $(a_{NbB2})*(a_{Ti}) = 1.95*10^{-3}$ for Nb_3Al $= 1.45*10^{-3}$ for Nb_2Al	Bordeline case-marginally compatible.
	(2)Kleppa's ΔH^{o}_{298} data for TiB_2: $(a_{NbB2})*(a_{Ti}) = 8.61*10^{-5}$ for Nb_3Al $= 6.42*10^{-5}$ for Nb_2Al	Compatible
TiB	Formation of NbB_2 and dissolution of Ti in matrix: Reaction: $\underline{Nb} + 2TiB = NbB_2 + 2\underline{Ti}$ $(a_{Ti})_{eq} = 0.085$ for Nb_3Al $= 0.073$ for Nb_2Al	Not compatible
VB	Formation of NbB_2 and dissolution of V in matrix: Reaction: $\underline{Nb} + 2VB = NbB_2 + 2\underline{V}$ $(a_V)_{eq} = 0.03$ for Nb_3Al $= 0.026$ for Nb_2Al	Not compatible
VB_2	Formation of NbB_2 and dissolution of V in matrix: Reaction: $\underline{Nb} + VB_2 = NbB_2 + \underline{V}$ $(a_V)_{eq} = 0.127$ for Nb_3Al $= 0.094$ for Nb_2Al	Not compatible
V_3B_2	Formation of NbB_2 and dissolution of V in matrix: Reaction: $\underline{Nb} + V_3B_2 = NbB_2 + 3\underline{V}$ $(a_V)_{eq} = 0.053$ for Nb_3Al $= 0.048$ for Nb_2Al	Not compatible

TABLE VIII (contd.)

Compatibility of Nb_3Al and Nb_2Al with borides at 1773

Boride	Mode of reaction	Comments on compatibility
V_2B_3	Formation of NbB_2 and dissolution of V in the matrix: Reaction: $3\underline{Nb} + 2V_2B_3 = 3NbB_2 + 4\underline{V}$ $(a_V)_{eq} = 0.053$ for Nb_3Al $= 0.048$ for Nb_2Al	Not compatible
ZrB_2	Formation of Al_2Zr and dissolution of NbB_2 in zrB_2: Reaction: $\underline{Nb}+2\underline{Al}+ZrB_2 = \underline{NbB_2}+Al_2Zr$ $(a_{NbB2})_{eq} = 9.86*10^{-4}$ for Nb_3Al $= 1.01*10^{-3}$ for Nb_2Al	Compatible

TABLE IX
Compatibility of $NbAl_3$ with borides at 1573 K

Boride	Mode of reaction	Comments on compatibility
AlB_{12}	Not stable in matrix-- NbB_2 is the stable boride.	Not compatible
CrB_2	Formation of NbB_2 and free Cr Reaction: $\underline{Nb} + CrB_2 = NbB_2 + Cr$	Not compatible
HfB_2	Formation of Al_2Hf and dissolution of NbB_2 in HfB_2 Reaction: $\underline{Nb}+2\underline{Al}+HfB_2 = \underline{NbB_2}+Al_2Hf$ $(a_{NbB2})_{eq} = 2.88*10^{-3}$	Compatible, probably borderline situation
LaB_6	Formation of NbB_2 and free La Reaction: $3\underline{Nb} + LaB_6 = 3NbB_2 + La$	Not compatible
NbB_2	Stable boride in the matrix	Compatible
ScB_2	Dissolution of Sc in matrix and of NbB_2 in ScB_2 Reaction: $\underline{Nb} + ScB_2 = \underline{NbB_2} + \underline{Sc}$ $(a_{NbB2})*(a_{Sc}) = 3.18*10^{-6}$	Compatible
TaB_2	Dissolution of Ta in matrix and of NbB_2 in TaB_2 Reaction: $\underline{Nb} + TaB_2 = \underline{NbB_2} + \underline{Ta}$ $(a_{NbB2})*(a_{Ta}) = 0.017$	Not compatible
TiB_2	Formation of TiAl and dissolution of NbB_2 in TiB_2 Reaction: $\underline{Nb}+\underline{Al}+TiB_2 = TiAl+\underline{NbB_2}$ $(a_{NbB2})_{eq} = 6.97*10^{-4}$	Compatible

TABLE IX (contd.)
Compatibility of $NbAl_3$ with borides at 1573

Boride	Mode of reaction	Comments on compatibility
TiB	Formation of NbB_2 and dissolution of Ti in matrix Reaction: $\underline{Nb} + 2TiB = NbB_2 + 2\underline{Ti}$ $(a_{Ti})_{eq} = 0.015$	Not compatible
VB	Formation of NbB_2 and dissolution of V in matrix Reaction: $\underline{Nb} + 2VB = NbB_2 + 2\underline{V}$ $(a_V)_{eq} = 0.011$	Not compatible
VB_2	Formation of NbB_2 and dissolution of V in matrix Reaction: $\underline{Nb} + VB_2 = NbB_2 + \underline{V}$ $(a_V)_{eq} = 0.03$	Not compatible
V_3B_2	Formation of NbB_2 and dissolution of V in matrix Reaction: $\underline{Nb} + V_3B_2 = NbB_2 + 3\underline{V}$ $(a_V)_{eq} = 0.011$	Not compatible
V_2B_3	Formation of NbB_2 and dissolution of V in matrix Reaction: $3\underline{Nb} + 2V_2B_3 = 3NbB_2 + 4\underline{V}$ $(a_V)_{eq} = 0.016$	Not compatible
ZrB_2	Formation of Al_2Zr and dissolution of NbB_2 in ZrB_2 Reaction: $\underline{Nb}+2\underline{Al}+ZrB_2 = Al_2Zr+\underline{NbB_2}$ $(a_{NbB2})_{eq} = 4.72*10^{-3}$	Borderline case, can be compatible if doped with small amount of Nb.

TABLE X

Compatibility of Nb_3Al and Nb_2Al with oxides at 1773 K

Oxide	Mode of reaction	Comments on compatibility
Al_2O_3	No reaction	Compatible
BeO	Formation of Al_2O_3 and dissolution of Be in the matrix Reaction: $2\underline{Al} + 3BeO = Al_2O_3 + 3\underline{Be}$ $(a_{Be})_{eq} = 6.2*10^{-4}$ for Nb_3Al $= 6.9*10^{-4}$ for Nb_2Al	Compatible
CaO	Formation of Al_2O_3 and dissolution of Ca in the matrix Reaction: $2\underline{Al} + 3CaO = Al_2O_3 + 3\underline{Ca}$ $(a_{Ca})_{eq} = 2.41*10^{-4}$ for Nb_3Al $= 2.66*10^{-4}$ for Nb_2Al	Compatible
CeO_2	Formation of Al_2O_3 and dissolution of Ce in matrix Reaction: $4\underline{Al}+3CeO_2 = 2Al_2O_3+3\underline{ce}$ $(a_{Ce})_{eq} = 8.18*10^{-3}$ for Nb_3Al $= 0.01$ for Nb_2Al	Not compatible; compatible if solubility of Ce in the matrix is negligible.
Cr_2O_3	Formation of Al_2O_3 and free Cr Reaction: $2\underline{Al}+Cr_2O_3 = Al_2O_3+2Cr$	Not compatible
Gd_2O_3	Formation of Al_2O_3 and dissolution of Gd in matrix Reaction: $2\underline{Al}+Gd_2O_3 = Al_2O_3+2\underline{Gd}$ $(a_{Gd})_{eq} = 3.25*10^{-5}$ for Nb_3Al $= 3.81*10^{-5}$ for Nb_2Al	Compatible
HfO_2	Formation of Al_2O_3 and dissolution of Hf in matrix Reaction: $4\underline{Al}+3HfO_2 = 2Al_2O_3+3\underline{Hf}$ $(a_{Hf}) = 5.59*10^{-5}$ for Nb_3Al $= 6.87*10^{-5}$ for Nb_2Al	Compatible
La_2O_3	Formation of Al_2O_3 and dissolution of La in matrix Reaction: $2\underline{Al}+La_2O_3 = Al_2O_3+2\underline{La}$ $(a_{La})_{eq} = 2.56*10^{-5}$ for Nb_3Al $= 3.01*10^{-5}$ for Nb_2Al	Compatible

TABLE X (contd.)
Compatibility of Nb_3Al and Nb_2Al with oxides

Oxide	Mode of reaction	Comments on compatibility
MgO (closed system)	Formation of Al_2O_3 and dissolution of Mg in matrix Reaction: $2\underline{Al}+3MgO = Al_2O_3+3\underline{Mg}$ $(a_{Mg})_{eq} = 3.01*10^{-3}$ for Nb_3Al $= 3.35*10^{-3}$ for Nb_2Al	Borderline case; probably compatible since solubility of Mg in matrix is likely to be negligible.
MgO (open system)	Formation of Al_2O_3 and magnesium gas Reaction: $2\underline{Al}+3MgO = Al_2O_3+3Mg(g)$ $(p_{Mg})_{eq} = 0.057$ for Nb_3Al $= 0.063$ for Nb_2Al	Not compatible
Sc_2O_3	Formation of Al_2O_3 and dissolution of Sc in matrix Reaction: $2\underline{Al}+Sc_2O_3 = Al_2O_3+2\underline{Sc}$ $(a_{Sc})_{eq} = 9.93*10^{-7}$ for Nb_3Al $= 1.16*10^{-6}$ for Nb_2Al	Compatible
TiO	Formation of Al_2O_3 and dissolution of Ti in matrix Reaction: $2\underline{Al}+3TiO = Al_2O_3+3\underline{Ti}$ $(a_{Ti})_{eq} = 0.029$ for Nb_3Al $= 0.032$ for Nb_2Al	Not compatible
TiO_2	Formation of Al_2O_3 and free Ti Reaction: $4\underline{Al}+3TiO_2 = 2Al_2O_3+3Ti$	Not compatible
Y_2O_3	Formation of Al_2O_3 and dissolution of Y in matrix Reaction: $2\underline{Al}+Y_2O_3 = Al_2O_3+2\underline{Y}$ $(a_Y)_{eq} = 6.14*10^{-7}$ for Nb_3Al $= 7.21*10^{-7}$ for Nb_2Al	Compatible
ZrO_2	Formation of Al_2O_3 and dissolution of Zr in matrix Reaction: $4\underline{Al}+3ZrO_2 = 2Al_2O_3+3\underline{Zr}$ $(a_{Zr})_{eq} = 9.4*10^{-6}$ for Nb_3Al $= 1.3*10^{-5}$ for Nb_2Al	Compatible

TABLE XI
Compatibility of $NbAl_3$ with oxides at 1573 K

Oxide	Mode of reaction	Comments on compatibility
Al_2O_3	No reaction	Compatible
BeO	Formation of Al_2O_3 and dissolution of Be in matrix Reaction: $2\underline{Al}+3BeO = Al_2O_3+3\underline{Be}$ $(a_{Be})_{eq} = 9.23*10^{-4}$	Compatible
CaO	Conditions just sufficient for formation of $3CaO.Al_2O_3$ and $CaAl_2$ Reaction: $8\underline{Al}+6CaO = 3CaO.Al_2O_3+3CaAl_2$	Not compatible
CeO_2	Formation of Al_2O_3 and Al_2Ce Reaction: $10\underline{Al}+3CeO_2 = 2Al_2O_3+3Al_2Ce$	Not compatible
Cr_2O_3	Formation of Al_2O_3 and free Cr Reaction: $2\underline{Al}+Cr_2O_3 = Al_2O_3+2Cr$	Not compatible
Gd_2O_3	Formation of Al_2O_3 and dissolution of Gd in matrix Reaction: $2\underline{Al}+Gd_2O_3 = Al_2O_3+2\underline{Gd}$ $(a_{Gd})_{eq} = 5.45*10^{-5}$	Compatible
HfO_2	Formation of Al_2O_3 and dissolution of Hf in matrix Reaction: $4\underline{Al}+3HfO_2 = 2Al_2O_3+3\underline{Hf}$ $(a_{Hf})_{eq} = 4.49*10^{-4}$	Compatible
La_2O_3	Formation of Al_2O_3 and dissolution of La in the matrix Reaction: $2\underline{Al}+La_2O_3 = Al_2O_3+2\underline{La}$ $(a_{La})_{eq} = 4.07*10^{-5}$	Compatible

TABLE XI (contd.)

Compatibility of $NbAl_3$ with oxides at 1573 K

Oxide	Mode of reaction	Comments on compatibility
MgO (open system)	Formation of Al_2O_3 and dissolution of Mg in the matrix Reaction: $2\underline{Al}+3MgO = Al_2O_3+3\underline{Mg}$ $(a_{Mg})_{eq} = 5.2*10^{-3}$	Probably compatible since solubility of Mg in $NbAl_3$ is likely to be negligible.
MgO (open system)	Formation of Mg gas and Al_2O_3 Reaction: $2\underline{Al}+3MgO = Al_2O_3+3Mg(g)$ $(p_{Mg})_{eq} = 0.032$	Not compatible
Sc_2O_3	Formation of A_2O_3 and dissolution of Sc in the matrix Reaction: $2\underline{Al}+Sc_2O_3 = Al_2O_3+2\underline{Sc}$ $(a_{Sc})_{eq} = 1.44*10^{-6}$	Compatible
SiO_2	Formation of Al_2O_3 and free Si Reaction: $4\underline{Al}+3SiO_2 = 2Al_2O_3+3Si$	Not compatible
TiO	Formation of Al_2O_3 and dissolution of Ti in matrix Reaction: $2\underline{Al}+3TiO = Al_2O_3+3\underline{Ti}$ $(a_{Ti})_{eq} = 0.094$	Not compatible
TiO_2	Formation of Al_2O_3 and free Ti Reaction: $4\underline{Al}+3TiO_2 = 2Al_2O_3+3Ti$	Not compatible
Y_2O_3	Formation of Al_2O_3 and dissolution of Y in matrix Reaction: $2\underline{Al}+Y_2O_3 = Al_2O_3+2\underline{Y}$ $(a_Y)_{eq} = 9.55*10^{-7}$	Compatible
ZrO_2	Formation of Al_2O_3 and Al_2Zr Reaction: $10\underline{Al}+3ZrO_2 = 2Al_2O_3+3Al_2Zr$	Not compatible

TABLE XII
Compatibility of Nb_3Al and Nb_2Al with nitrides at 1773 K

Nitride	Mode of reaction	Comments on compatibility
AlN	Nb_2N is the stable nitride in matrix	Not compatible
BN	Formation of Nb_2N and NbB_2 Reaction: $5\underline{Nb}+2BN = 2Nb_2N+NbB_2$	Not compatible
HfN	Formation of Al_2Hf and dissolution of Nb_2N in HfN Reaction: $2\underline{Nb}+2\underline{Al}+HfN = \underline{Nb2N}+Al_2Hf$ $(a_{Nb2N})_{eq} = 2.39*10^{-3}$ for Nb_3Al $= 2.45*10^{-3}$ for Nb_2Al	Borderline case; can be made compatible if doped with small amount of Nb.
LaN	Dissolution of La in matrix and of Nb_2N in LaN Reaction: $2\underline{Nb}+LaN = \underline{Nb2N}+\underline{La}$ $(a_{Nb2N})*(a_{La}) = 0.421$ for Nb_3Al $= 0.233$ for Nb_2Al	Not compatible
Si_3N_4	Formation of Nb_2N and free Si Reaction: $8\underline{Nb}+Si_3N_4 = 4Nb_2N+3Si$	Not compatible
TaN	Dissolution of Ta in matrix and of Nb_2N in TaN Reaction: $2\underline{Nb}+TaN = \underline{Nb2N}+\underline{Ta}$ $(a_{Nb2N})*(a_{Ta}) = 0.628$ for Nb_3Al $= 0.348$ for Nb_2Al	Not compatible
TiN	Dissolution of Ti in matrix and of Nb_2N in TiN Reaction: $2\underline{Nb}+TiN = \underline{Nb2N}+\underline{Ti}$ $(a_{Nb2N})*(a_{Ti}) = 5.43*10^{-3}$ for Nb_3Al $= 3.01*10^{-3}$ for Nb_2Al	Borderline case; can be made compatible if small amount of Ti is dissolved in alloy.
ZrN	Formation of Al_2Zr and dissolution of Nb_2N in ZrN Reaction: $2\underline{Nb}+2\underline{Al}+ZrN = \underline{Nb2N}+Al_2Zr$ $(a_{Nb2N})_{eq} = 8.13*10^{-3}$ for Nb_3Al $= 8.35*10^{-3}$ for Nb_2Al	Borderline case; compatible if doped with small amount of Nb.

TABLE XIII
Compatibility of $NbAl_3$ with nitrides at 1573 K

Nitride	Mode of reaction	Comments on compatibility
AlN	Stable nitride in matrix	Compatible
BN	Formation of AlN and NbB_2 Reaction: $\underline{Nb}+2\underline{Al}+2BN = NbB_2+2AlN$	Not compatible
HfN	Formation of Al_2Hf and dissolution of AlN in HfN Reaction: $3\underline{Al}+HfN = Al_2Hf+\underline{AlN}$ $(a_{AlN})_{eq} = 0.023$	Not compatible; compatible if doped with small amount of Al
LaN	Formation of AlN and $LaAl_2$ Reaction: $3\underline{Al}+LaN = AlN+LaAl_2$	Not compatible
Si_3N_4	Formation of AlN and free Si Reaction: $4\underline{Al}+Si_3N_4 = 4AlN+3Si$	Not compatible
TaN	Dissolution of Ta in matrix and of AlN in TaN Reaction: $\underline{Al}+TaN = \underline{AlN}+\underline{Ta}$ $(a_{AlN})*(a_{Ta}) = 0.416$	Not compatible
TiN	Formation of TiAl and dissolution of AlN in TiN Reaction: $2\underline{Al}+TiN = TiAl+\underline{AlN}$ $(a_{AlN}) = 4.64*10^{-3}$	Borderline case; probably compatible
ZrN	Formation of Al_2Zr and dissolution of AlN in ZrN Reaction: $3\underline{Al}+ZrN = Al_2Zr+\underline{AlN}$ $(a_{AlN})_{eq} = 0.082$	Not compatible

TABLE XIV

Compatibility of Nb_3Al, Nb_2Al, and $NbAl_3$ with silicides
(Calculations for Nb_3Al and Nb_2Al performed at 1773)
(Calculations for $NbAl_3$ performed at 1573 K)

Silicide	Mode of reaction	Comments on compatibility
Cr_3Si	Formation of Nb_5Si_3 and free Cr Reaction: $5\underline{Nb}+3Cr_3Si = Nb_5Si_3+9Cr$	Not compatible
Cr_5Si_3	Formation of Nb_5Si_3 and free Cr Reaction: $5\underline{Nb}+Cr_5Si_3 = Nb_5Si_3+5Cr$	Not compatible
Mo_3Si	Formation of Nb_5Si_3 and free Mo Reaction: $5\underline{Nb}+3Mo_3Si=Nb_5Si_3+9Mo$	Not compatible
Mo_5Si_3	Formation of Nb_5Si_3 and free Mo Reaction: $5\underline{Nb}+Mo_5Si_3=Nb_5Si_3+5Mo$	Not compatible
$MoSi_2$	Formation of Nb_5Si_3 and free Mo Reaction: $10\underline{Nb}+3MoSi_2=2Nb_5Si_3+3Mo$	Not compatible
Nb_5Si_3	No reaction	Compatible
$NbSi_2$	Formation of Nb_5Si_3 Reaction: $7\underline{Nb}+3NbSi_2 = 2Nb_5Si_3$	Not compatible
Ta_2Si	Formation of Nb_5Si_3 and free Ta Reaction: $5\underline{Nb}+3Ta_2Si = Nb_5Si_3+6Ta$	Not compatible
Ta_5Si_3	Formation of Nb_5Si_3 and free Ta Reaction: $5\underline{Nb}+Ta_5Si_3 = Nb_5Si_3+5Ta$	Not compatible
$TaSi_2$	Formation of Nb_5Si_3 and free Ta Reaction: $10\underline{Nb}+3TaSi_2 = 2Nb_5Si_3+3Ta$	Not compatible
Ti_5Si_3	Formation of Nb_5Si_3 and dissolution of Ti in matrix Reaction: $5\underline{Nb}+Ti_5Si_3 = Nb_5Si_3+5\underline{Ti}$ $(a_{Ti})_{eq} = 0.152$ for Nb_3Al $= 0.113$ for Nb_2Al $= 0.039$ for $NbAl_3$	Not compatible

TABLE XIV (contd.)

Compatibility of Nb_3Al and Nb_2Al with silicides at 1773 K

Silicide	Mode of reaction	Comments on compatibility
TiSi	Nb_3Al and Nb_2Al: Formation of Nb_5Si_3 and free Ti Reaction: $5\underline{Nb}+3TiSi = Nb_5Si_3+3Ti$	Not compatible
	$NbAl_3$: Formation of Nb_5Si_3 and dissolution of Ti in matrix Reaction: $5\underline{Nb}+3TiSi = Nb_5Si_3+3\underline{Ti}$ $(a_{Ti})_{eq} = 0.81$	Not compatible
V_3Si	Formation of Nb_5Si_3 and free V Reaction: $5\underline{Nb}+3V_3Si = Nb_5Si_3+9V$	Not compatible
V_5Si_3	Formation of Nb_5Si_3 and dissolution of V in matrix Reaction: $5\underline{Nb}+V_5Si_3 = Nb_5Si_3+5\underline{V}$ $(a_V)_{eq} = 0.237$ for Nb_3Al $= 0.176$ for Nb_2Al	Not compatible
VSi_2	Formation of Nb_5Si_3 and free V Reaction: $10\underline{Nb}+3VSi_2 = 2Nb_5Si_3+3V$	Not compatible
W_5Si_3	Formation of Nb_5Si_3 and free W Reaction: $5\underline{Nb}+W_5Si_3 = Nb_5Si_3+5W$	Not compatible
WSi_2	Formation of Nb_5Si_3 and free W Reaction: $10\underline{Nb}+3WSi_2 = 2Nb_5Si_3+3W$	Not compatible
Zr_2Si	Formation of Nb_5Si_3 and Al_2Zr Reaction: $5\underline{Nb}+12\underline{Al}+3Zr_2Si=Nb_5Si_3+6Al_2Zr$	Not compatible
Zr_5Si_3	Formation of Nb_5Si_3 and Al_2Zr Reaction: $5\underline{Nb}+10\underline{Al}+Zr_5Si_3=Nb_5Si_3+5Al_2Zr$	Not compatible
ZrSi	Nb_3Al: Formation of Nb_5Si_3 and free Zr Reaction: $5\underline{Nb}+3ZrSi = Nb_5Si_3+3Zr$	Not compatible
	Nb_2Al and $NbAl_3$: Formation of Nb_5Si_3 and Al_2Zr Reaction: $5\underline{Nb}+6\underline{Al}+3ZrSi=Nb_5Si_3+3Al_2Zr$	Not compatible

TABLE XV

Compatibility of Nb_3Al, Nb_2Al, and $NbAl_3$ with Engel-Brewer compounds
(Calculations for Nb_3Al and Nb_2Al performed at 1773 K)
(Calculations for $NbAl_3$ performed at 1573 K)

Engel-Brewer compound	Mode of reaction	Comments on compatibility
HfPt	Nb_3Al and Nb_2Al: Formation of AlPt and dissolution of Hf in the matrix Reaction: $\underline{Al}$+HfPt = AlPt+$\underline{Hf}$ $(a_{Hf})_{eq} = 3.07*10^{-3}$ for Nb_3Al $= 3.62*10^{-3}$ for Nb_2Al	Borderline case, probably compatible
	$NbAl_3$: Formation of AlPt and Al_2Hf Reaction: 3$\underline{Al}$+HfPt = AlPt+Al_2Hf	Not compatible
$HfPt_3$	Formation of AlPt and free Hf Reaction: 3$\underline{Al}$+$HfPt_3$ = 3AlPt+Hf	Not compatible
$NbCr_2$	Dissolution of Cr in matrix Reaction: $\underline{Nb}$+2$\underline{Cr}$ = $NbCr_2$ $(a_{Cr})_{eq} = 0.458$ for Nb_3Al $= 0.531$ for Nb_2Al $= 0.748$ for $NbAl_3$	Not compatible
TiIr	Formation of AlIr and free Ti Reaction: $\underline{Al}$+TiIr = AlIr+Ti	Not compatible
$TiIr_3$	Formation of AlIr and free Ti Reaction: 3$\underline{Al}$+$TiIr_3$ = 3AlIr+Ti	Not compatible
TiPt	Formation of AlPt and free Ti Reaction: $\underline{Al}$+TiPt = AlPt+Ti	Not compatible
$TiPt_3$	Formation of AlPt and free Ti Reaction: 3$\underline{Al}$+$TiPt_3$ = 3AlPt+Ti	Not compatible
$ZrIr_3$	Nb_3Al and Nb_2Al: Formation of AlIr and Al_2Zr Reaction:5$\underline{Al}$+$ZrIr_3$ = 3AlIr+Al_2Zr	Not compatible
	$NbAl_3$: Formation of AlIr and free Zr Reaction: 3$\underline{Al}$+$ZrIr_3$ = 3AlIr+Zr	Not compatible

TABLE XV (contd.)

Compatibility of Nb_3Al, Nb_2Al, and $NbAl_3$ with Engel-Brewer compounds

Engel-Brewer compound	Mode of reaction	Comments on compatibility
ZrPt	Nb_3Al: Formation of AlPt and dissolution of Zr in matrix Reaction: $\underline{Al}+ZrPt = AlPt+\underline{Zr}$ $(a_{Zr})_{eq} = \overline{0}.034$	Not compatible, compatible if solubility of Zr in Nb_3Al is low.
	Nb_2Al and $NbAl_3$: Formation of AlPt and Al_2Zr Reaction: $3\underline{Al}+ZrPt = AlPt+Al_2Zr$	Not compatible
$ZrPt_3$	Formation of AlPt and free Zr Reaction: $3\underline{Al}+ZrPt_3 = 3AlPt+Zr$	Not compatible

APPENDIX A
THERMODYNAMIC DATA FOR COMPOUNDS

Standard Gibbs Energies of Formation for Carbides

Carbide	$-\Delta G_f^o$ at 1573 K (kCal/mol)	$-\Delta G_f^o$ at 1773 K (kCal/mol)	Reference
Al_4C_3	27.46	22.84	1
B_4C	13.42	12.99	1
HfC	52.22	51.79	1
Mo_2C	12.86	13.06	1
NbC	32.70	32.70	1
Nb_2C	41.93	41.41	1
SiC	12.92	12.60	1
TaC	33.71	33.87	1
Ta_2C	47.44	47.45	1
TiC	39.48	38.79	1
V_2C	34.18	33.99	1
VC	21.01	20.49	1
W_2C	22.33	24.71	1
WC	8.21	8.10	1
ZrC	43.46	42.96	1

APPENDIX A (contd.)

Standard Gibbs Energies of Formation for Borides

Boride	$-\Delta G_f^o$ at 1573 K (kCal/mol)	$-\Delta G_f^o$ at 1773 K (kCal/mol)	Reference
AlB_{12}	48.79	48.29	1
CrB_2	25.40	25.20	1
HfB_2	75.80	75.24	1
LaB_6	95.60*	95.60*	2
NbB_2	38.34	38.07	1
ScB_2	73.40*	73.40*	3
TaB_2	46.41	45.96	1
TiB_2	60.02	58.91	1
	71.02**	69.91**	3
TiB	29.89	27.15	1
VB	31.07	30.80	1
VB_2	44.72	44.20	1
V_3B_2	68.43	67.87	1
V_2B_3	76.48	75.70	1
ZrB_2	69.77	68.41	1

---

* ΔG_f^o is taken to be the same as ΔH_{298}^o

** ΔH_{298}^o for TiB_2 taken from reference 4, rest of thermodynamic data taken from ref. 1.

APPENDIX A (contd.)

Standard Gibbs Energies of Formation for Oxides

Oxide	$-\Delta G_f^o$ at 1573 K (kCal/mol)	$-\Delta G_f^o$ at 1773 K (kCal/mol)	Reference
Al_2O_3	280.08	264.5	1
BeO	108.89	104.02	1
CaO	112.46	107.15	1
CeO_2	182.87	172.96	1
Cr_2O_3	172.01	159.96	1
Gd_2O_3	327.04	313.70	1
HfO_2	198.59	190.54	1
La_2O_3	321.96	308.49	1
MgO	97.85	88.08	1
Sc_2O_3	345.38	331.41	1
SiO_2	150.92	142.17	1
TiO	94.49	90.47	1
TiO_2	157.53	149.07	1
Y_2O_3	347.96	334.79	1
ZrO_2	191.71	183.19	1

Standard Gibbs Energies of Formation for Nitrides

Nitride	$-\Delta G_f^o$ at 1573 K (kCal/mol)	$-\Delta G_f^o$ at 1773 K (kCal/mol)	Reference
AlN	34.51	28.90	1
BN	27.11	23.06	1
HfN	56.01	52.08	1
LaN	30.93	25.64	1
Nb_2N	28.64	24.86	1
Si_3N_4	53.94	36.71	1
TaN	27.86	24.23	1
TiN	45.38	40.97	1
ZrN	52.12	47.77	1

APPENDIX A (contd.)

Standard Gibbs Energies of Formation for Silicides

Silicide	$-\Delta G_f^o$ at 1573 (kCal/mol)	$-\Delta G_f^o$ at 1773 K (kCal/mol)	Reference
Cr_3Si	24.28	23.54	1
Cr_5Si_3	58.64	57.54	1
Mo_3Si	27.88	27.13	1
Mo_5Si_3	76.66	74.91	1
$MoSi_2$	30.73	29.29	1
Nb_5Si_3	112.75	111.52	1
$NbSi_2$	30.75	29.13	1
Ta_2Si	31.30	30.88	1
Ta_5Si_3	85.08	83.90	1
$TaSi_2$	19.98	17.64	1
Ti_5Si_3	140.81	138.94	1
TiSi	30.74	30.05	1
V_3Si	33.31	31.95	1
V_5Si_3	128.00	131.18	1
VSi_2	35.13	34.44	1
W_5Si_3	42.48	41.97	1
WSi_2	19.44	17.77	1
Zr_2Si	49.06	47.93	1
Zr_5Si_3	136.27	133.12	1
ZrSi	35.83	34.81	1

APPENDIX A (contd.)

Standard Gibbs Energies of Formation for Engel-Brewer Compounds

Gibbs free energies of formation for most of the Engel-Brewer compounds have been measured at one temperature. Therefore, for these compounds, G_f will be assumed to be the same at other temperatures. The table below gives the G_f values for the Engel-Brewer compounds and the temperature at which measurements were made.

Engel-Brewer compound	$-\Delta G_f^o$ (kCal/mol)	Temperature (K)	Reference
AlIr	34.2	1500	4
AlPt	49.2	1500	4
HfPt*	50.64	1473	5
$HfPt_3$	97.35	1300	6
$NbIr_3$	32.00	1770	7
TiIr	39.79	2000	8
$TiIr_3$	56.02	2000	8
TiPt*	34.38	1473	5
$TiPt_3$	71.3	1300	9
$ZrIr_3$	62.8	1873	8
ZrPt*	42.17	1473	5
$ZrPt_3$	91.74	1300	6

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* Reference 6 gives ΔH_f^o at 1473 K. ΔG_f^o calculated by assuming the entropy of mixing to be equal to -2.5 cal mol^{-1} K^{-1} which is the same as that for TiIr (ref. 7).

APPENDIX A (contd.)

Standard Gibbs Energies of formation for other intermetallics

Intermetallic compound	$-\Delta G_f^o$ at 1573 K (kCal/mol)	$-\Delta G_f^o$ at 1773 K (kCal/mol)	Reference
Al_2Zr^*	37.95	37.58	10
Al_2Hf^{**}	37.95	37.58	-
$CaAl_2(l)$	43.91	43.73	1
$CeAl_2$	33.51	31.63	1
$Cr_{.41}Al_{.59}{}^{***}$	4.84	4.73	10
$LaAl_2$	23.84	20.98	1
Mo_3Al	16.01	16.22	11
Mo_3Al_8	41.81	41.43	11
$NbCr_2$	6.31	6.63	1
TiAl	12.85	11.81	1
$V_{.395}Al_{.605}$	0.65	0.65	10

---

*. ΔG for reaction $2Al(s) + Zr(s) = Al_2Zr$ measured at 1023 K. The G for this reaction is assumed to be the same at other temperatures.

**. ΔG_f^o assumed to be the same as that of Al_2Zr.

***. ΔG for reaction $0.41Cr(s)+0.59Al(s) = Cr_{.41}Al_{.59}$ measured at 1273 K. The ΔG for this reaction is assumed to be the same at other temperatures.

APPENDIX A (contd.)

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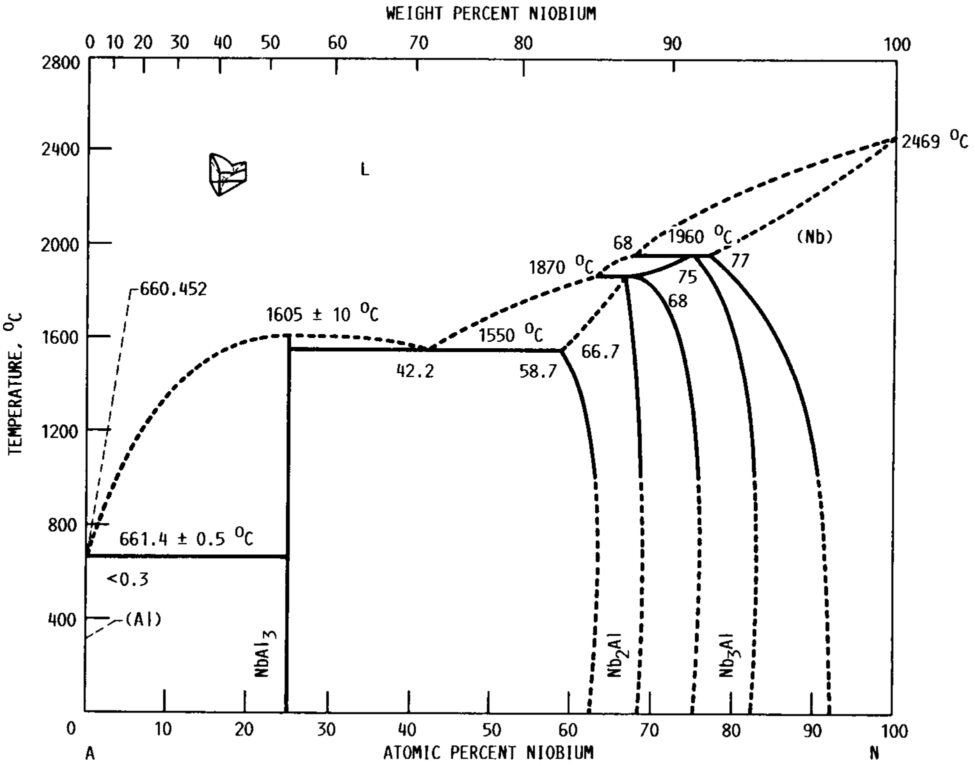

FIGURE 1. - Nb - Al PHASE DIAGRAM. (FROM REF. 3).

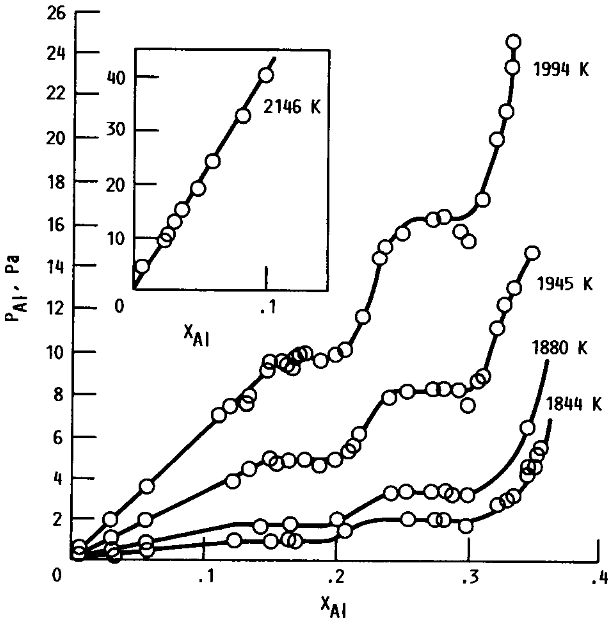

FIGURE 2. - VAPOR PRESSURE OF Al AS A FUNCTION OF TEMPERATURE AND ALLOY COMPOSITION. (FROM REF. 5).

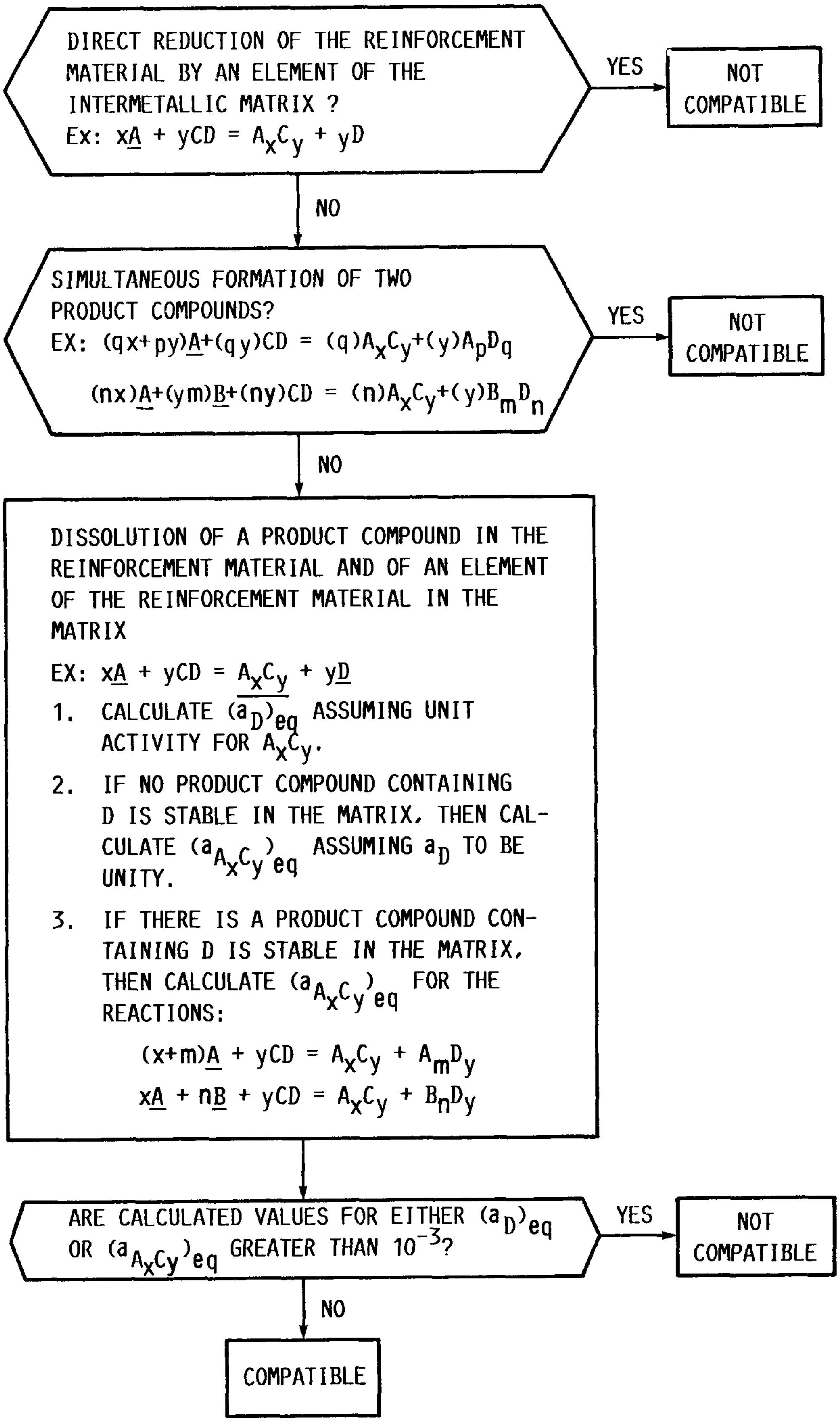

FIGURE 3. - COMPATIBILITY CALCULATIONS - SEQUENCE OF STEPS.

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16. Abstract
Chemical compatibility of several reinforcement materials with three niobium aluminides, Nb_3Al, Nb_2Al, and $NbAl_3$, were examined from thermodynamic considerations. The reinforcement materials considered in this study include carbides, borides, nitrides, oxides, silicides, and Engel-Brewer compounds. Thermodynamics of the Nb-Al system were reviewed and activities of Nb and Al were derived at desired calculation temperatures. Criteria for chemical compatibility between the reinforcement material and Nb-Al compounds have been defined and several chemically compatible reinforcement materials have been identified.

17. Key Words (Suggested by Author(s))
Niobium; Aluminides; Fibers; Composites; Thermodynamics

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