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Our primary goal is to study and develop alloying concepts for understanding intermetallic alloys as derived from a highly precise quantum mechanical approach. Thus, a major part of our effort is to study and determine ductilizing effects and to work closely with experimental efforts to evaluate the applicability of the theoretical approach to alloy design. Specifically we have studied a number of materials problems to obtain first principles information of relevance to alloy stability and design of structural materials. Fundamental information has been obtained about the structural and electronic properties in order to predict stable and metastable phases and how alloying affects bonding, crystal order and crystal symmetry. Our approach addresses questions of a metallurgical nature, such as phase stability, crystal structure, equilibrium lattice constants, and mechanical properties. For the ordered compounds, tailoring the chemistry of these alloys to obtain higher symmetry (and thus more ductile) crystalline phases is extremely important. The research seeks to explore a new capability for modelling materials and their properties on the computer which have not yet been made in practice.

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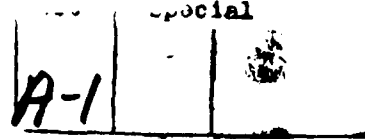
**Quantum Mechanical Approach to Understanding
Structural, Electronic and Mechanical Properties of
Intermetallics**

by

A.J. Freeman, Principal Investigator

ABSTRACT

The primary goal of the AFOSR supported research is to study and develop alloying concepts for understanding intermetallic alloys as derived from a first principles quantum mechanical approach. Thus, a major part of our effort is to study and determine ductilizing effects of alloying elements in several intermetallic compounds and to work closely with experimental efforts to evaluate the applicability of the theoretical approach to alloy design. Specifically, highly precise all-electron quantum mechanical electronic structure methods were applied to the study of a number of materials problems in order to obtain from first principles information of relevance to alloy stability and design of structural materials. Using state-of-the-art all-electron self-consistent total energy methods which give precise solutions of the local density equations, fundamental information has been sought about the structural and electronic properties of these alloys in order to predict stable and metastable phases and how alloying affects bonding, crystal order and crystal symmetry. The first principles approach used here addresses questions of a metallurgical nature, such as phase stability, crystal structure, equilibrium lattice constants, and mechanical properties. For the ordered compounds, tailoring the chemistry of these alloys to obtain higher symmetry (and thus more ductile) crystalline phases is extremely important. The research seeks to explore a new capability for modelling materials and their properties on the computer which have not yet been made in practice.



I. INTRODUCTION

It is now well recognized that modern aerospace applications demand materials that are stiffer, stronger and lighter than those used in the last twenty years. Further, the development of these materials is essential because of the growing challenges facing aerospace engineers who must design advanced, reduced-weight vehicles which feature both increased economy and performance. Material properties such as elastic anisotropy must be fully utilized in vehicles designed for high Mach speeds. Along with advances expected in structural materials, high temperature-resistant components (i.e., for jet engines) are also of considerable importance because weight reduction together with increased high temperature performance can increase engine efficiency, thereby achieving a high thrust to weight ratio.

Considerable effort has gone into the development of ordered alloys for high temperature structural applications especially in the last decade. As emphasized by Lipsitt, Dimiduk and others, "intermetallic compounds are particularly suited to these aerospace needs because of two properties which derive from the fact that they possess ordered structures. Modulus retention with temperature in these materials is particularly high because of the strong A-B bonding. In addition, a number of high temperature properties which depend on diffusive mechanisms are improved because of the generally high activation energy required for diffusion in ordered alloys. Included in this category are static strength retention, creep/stress-rupture, and fatigue resistance. Finally, in the case of aluminides, the oxidation resistance is particularly good because all of these materials contain a large aluminum reservoir. In many intermetallics strong A-B bonding also results in low temperature brittleness, although the exact mechanism of the ductile-brittle transition seems to be different in every case. It is necessary for the alloy developer to ease the problem of minimal low temperature ductility without destroying the valuable ordered structure which provides the high temperature strength and stiffness."

The driving force behind our research is the recognition that technological advances depend strongly on a thorough understanding of the thermodynamic, mechanical, and electronic properties of materials. These, in turn, depend on our predictive ability regarding these properties. It is particularly the understanding of the structure and stability of the phases of compounds and alloys which is of vital importance to materials science and technology. Such an understanding is starting to emerge from our first steps into carrying out all-electron quantum

mechanical investigations on materials of aerospace interest. Briefly put, our emphasis has been on obtaining an understanding of the effects of alloying on bonding, crystal structure and phase stability of structural materials and to use this information to help design new alloy systems. It should be emphasized that this work is carried out in close collaboration with the experimental effort at Wright-patterson AFB, at GE Aircraft Engines, Cincinnati, and elsewhere.

II. PROGRESS

We have previously reported on our progress made in considering a number of problems, principally the structural stability and structural properties of Ni_3Al . One of the chief accomplishments of that work was to make use of our understanding of the phase stability in a practical way. To this end, we have studied the density of states for the different structures and have found that there is a correlation between the stability and the density of states at the Fermi energy in that the energetically favorable atomic arrangement of Ni_3Al leads to a low density of states at the Fermi energy. This appears to be a universal feature in all the aluminides we have studied and, it turns out, permits us to make predictions about the possible stabilization of the cubic L_{12} phase by means of ternary additions.

As a next step, we considered the site preference in solid solution strengthening upon addition of V to Ni_3Al first by considering the separate studies of Ni_3Al and Ni_3V . We found for the pure systems that the lattice constants and bulk modulus were in good agreement with experiment and other calculations. Further, with ternary additions considered using model calculations we found that the L_{12} -like Ni_3Al can dissolve up to 50% V replacing Al in an ordered way and still retain the L_{12} -like structure with a lower energy than in the DO_{22} -like structure. In addition, we found a slight hardening effect caused by the V when added to Ni_3Al . We then did a band analysis to determine the role of density of states (DOS) in stabilizing intermetallics - notably in the role of the V additions to Ni_3Al . Among other results we found that for $\text{Ni}_3(\text{Al,V})$ in the L_{12} -like structure, there are enough valence electrons due to the V addition to bring the Fermi level to a position just below the bonding d-d hybrid states. Thus, the valence electrons fill all the bonding states and leave all the anti-bonding states empty; therefore, the strongest bonding occurs in $\text{Ni}_3(\text{Al,V})$ in the L_{12} -like structure. For this reason, it is also expected, from the rigid band sense, that Ti, Zr,

Hf, Nb, Ta, Si and Ge, will stabilize the $L1_2$ structure in Ni_3Al in much the same way as V, and possibly preferentially occupy Al sites.

We next applied some of this knowledge and methodology to understand the stabilization of high temperature structural materials in highly ductile phases. A prime example was our investigation of the electronic structure and cohesive properties of $ZrAl_3$ in the metastable $L1_2$ structure using the total energy local density linear muffin tin orbital approach. We follow the above described procedure of first determining the density of states at the Fermi energy as a way of stabilizing the cubic $L1_2$ phase of $ZrAl_3$. The results suggested that ternary additions like Li or Mg would lower E_F into the minimum in the DOS and hence stabilize the $L1_2$.

A. Structural Phase Stability of Titanium Aluminides

Most recently, we have initiated an in-depth study of the structural phase stability and electronic properties of several TiAl intermetallics (Ti_3Al , $TiAl$, and $TiAl_3$). To begin with, we studied the properties of pure Ti metal and have demonstrated that the hcp phase is lower than the bcc and fcc structures. An examination of the density of states at the Fermi energy for the three structures shows, once again, that the $N(E_F)$ is lowest for the hcp structure.

For the three TiAl compounds studied using our all-electron total energy approach, we find calculated equilibrium lattice constants in quite good agreement with experiment; the heat of formation and the bulk modulus also agree fairly well with the experimental results. Some of these results are presented in Table I. In all cases for the stable phase of the compounds, the Fermi energy is on the bonding side of the DOS curve and a lower DOS value appears again at the Fermi energy in agreement with our earlier studies cited above. This means that we may now have a good method for predicting which ternary additions would stabilize the $L1_2$ phase in $TiAl_3$ and in Ti_3Al . Some of these insights and predictions are now being fed to our experimental collaborators.

B. Combined Statistical Mechanical and Electronic Structure Approach to First Principles Determination of Alloy Phase Diagrams.

Stimulated by the complexity of alloy phase diagrams of the intermetallics, notably Ti-Al, we have undertaken a first step towards the calculation of the phase diagrams of binary alloys entirely from first principles. This has been a long-sought and important goal (which started with the work of Kikuchi). In our

approach, we start from a local density total energy supercell formulation. After constructing the grand partition function which permits the determination of the entropy from our calculated total electronic energies, we are, in principle, able to obtain all thermodynamic quantities. While this approach faces the same problem as obtaining the entropy in cluster variational methods, since one is presently restricted to relatively small unit cells, there are a number of important advantages: (1) solid solution and ordered phases can be calculated with the same numerical method and precision; (2) local environment effects such as charge transfer and chemical bonding are accurately described; (3) any crystal structure for which the total energy has been calculated can be easily included in the grand partition function; (4) the model is self-contained and only needs the total energy; and (5) no fitting and no breaking into pairwise interactions is necessary.

The result is a combined statistical mechanical and electronic structure approach which shows some promise. It should be emphasized that the grand partition function is constructed from volume dependent internal energies obtained from local density total energy supercell calculations. The illustrative results of first calculations for the Al-Li system show: (i) structural properties versus concentration in very good agreement with experiment and (ii) features on the Al rich side of the phase diagram of the fcc solid solution which are important for alloy formation. Since we are limited to small supercells at present, our method should only be applied to regions in experimentally known phase diagrams where complicated structures do not occur and where concentration waves with long wave lengths are not important. Within these restrictions, it appears that our combined statistical, mechanical and electronic structure method shows promise for studying alloy phase diagrams entirely from first principles

C. A First Principles Calculation of Phase Equilibria in the Aluminium Lithium System

We have initiated a collaborative program with Prof. D. de Fontaine and his group at the Department of Materials Science and Engineering, University of California, Berkeley to calculate phase equilibria. As a first case we have jointly studied the (metastable) equilibria in the aluminum-lithium system. This system has attracted considerable attention due to the technical importance of metastable Al_3Li precipitation hardening in Al-rich Al-Li alloys. Since this work has just been submitted we give some details here.

First principles approaches for the study of phase transformations, which do not require accurate experimental data, are of special interest in the case of the Al-Li system because of the difficulties encountered with experimental determinations of the metastable phase boundaries. Furthermore, ab initio approaches have the advantage of providing a deeper understanding of the underlying physics. As emphasized above, in the last decade the prediction of structural stabilities of phases at $T = 0$ K, has become possible through accurate electronic band structure computations based on the local electronic density functional theory. Only recently have first principles approaches become feasible for computation of phase stability away from $T = 0$ K, and schemes such as the TB-CPA-GPM-CVM and total energy - direct inversion - CVM are yielding increasingly realistic results. In our work, the second method, involving very accurate FLAPW total energy computations, have been employed.

In our total energy approach the total energies of a series of ordered compounds are calculated by our accurate electronic band structure method. Then it is assumed (following Kikuchi) that the formation energies (or total energies) can be expressed as the sum of the products of the cluster interactions and the cluster correlation functions. Because the cluster correlation functions of perfectly ordered compounds are solely determined by the crystal structure in question, one can obtain the cluster interactions if the total energies for a set of ordered compounds are known. The cluster interactions are given by the product of the inverse cluster correlation matrix and the total energy vector, hence we call this the "direct inversion method" - which has recently gained notable popularity.

The cluster interactions are introduced in a model (in this case the tetrahedron CVM) that provides configurational free energies by evaluating the statistical part of alloying. The configurational free energies of various phases can be complemented with free energy contributions from other sources, such as elastic, or magnetic effects, to yield total free energies which in turn are then used in procedures outlined by Gibbs to obtain a phase diagram.

More specifically, the truly ab initio computation of the solid state equilibria in the Al-Li system was found, on many salient points, to be in agreement with experimental findings, such as: 1) The correct prediction that fcc Al is much more stable than bcc Al; 2) That close to absolute zero temperature, the fcc structure is more stable than the bcc structure for Li, and that there is a small difference in the lattice stability of those two structures; 3) That the B32 structure

is much more stable than the B2 structure for the equi-atomic alloy; 4) The fact that the free energy of the Al_3Li - L_{12} phase is only just above the common tangent between the Al-rich solid solution and the B32 phase at ambient temperatures indicating the meta-stability of the Al_3Li - L_{12} phase; 5) That there is a relatively high solubility of Li in fcc Al which decreases with lower temperatures and the very small solubility of Al in both fcc and bcc Li; 6) The fact that the AlLi phase (B32) metals before disordering takes place; 7) The prediction of the correct order of magnitude for the critical temperature of the metastable Al_3Li - L_{12} phase; 8) The influence of excess Li on the lattice parameter of the B32 phase is shown to be in good agreement with experiment.

When empirical data was added, such as a simple concentration dependent vibrational entropy and a regular solution free energy for the liquid, more correspondences with the experimental phase diagram were observed, such as: 9) The occurrence of eutectics at both the Al- and the Li - rich sides of the phase diagrams. The cause of the deviations of the eutectic temperatures with respect to the experimental values was found and attributed to the form of the free energy expression for the liquid; 10) The B32 phase was found to melt congruently and a peritectic was observed at about 70 at% Li, between the eutectic at the Li-rich side and the melting point of the B32 phase. A few shortcomings were that a wide two phase region between the Al-rich solid solution and the Al_3Li - L_{12} phase could be found and the fact that the complex Al_4Li_9 (mC26, B2/m) and Al_2Li_3 (hR5, R3m) phases could not at present be included in this study. Although a feasible first principles formalism of the vibrational entropy is still lacking and the description of the liquid phase needs to be improved upon, first principles studies of phase equilibria were found to be feasible and useful. As a next step, we propose to study phase equilibria in the Ti-Al system.

D. Interfacial Properties of Intermetallics: (001) APB Energy of Ni_3Al .

Finally, we have started some first principles studies of the mechanical properties of the intermetallic compounds. Because of their importance in understanding the high temperature properties of Ni_3Al , we have calculated from first principles the energy of formation of an antiphase boundary (APB). Two different approaches were used: (i) a thin film method and (ii) a supercell method. In the supercell approach, this required 16 atoms per supercell and in the thin film approach we set up a comparison of the total energy of the ordered single

phase Ni_3Al with a 13 layer film. Surprisingly, both methods gave the same results, namely, $E = 140 \pm \text{erg/cm}^2$ - in very good agreement with the experimental result of Veyssiere et al.. We are presently also analyzing these results in terms of our ability to compare charge densities so as to better understand the interface. As a next step we will be undertaking a similar calculation of the (111) APB in Ni_3Al .

E. Ductilization of Intermetallics

Recently the AFOSR has funded the proposal by the GE group to work closely with this effort at developing the experimentally verifying alloying concepts derived from first principles that will facilitate development of new engineering materials based on intermetallic compounds. Clearly the use of low density intermetallic compounds, while advantageous, still has major problems - such as with NiAl which has very poor ductility which must be improved for aircraft engine application.

As a first step, we have been trying to understand the intrinsic brittleness of NiAl at room temperature of this otherwise promising material. Deformation experiments have shown that the nature of slip is $\langle 001 \rangle \{110\}$ in NiAl , which implies that only 3 independent slip systems exist. As the independent slip systems are orthogonal, there are no cross slips and therefore, von Mises criterion for ductility is not satisfied. Since the Burgers vectors in the disordered bcc structure are $1/2\langle 111 \rangle$, it is quite reasonable to believe that the ductility might be improved if it were to show $1/2\langle 111 \rangle$ type slip by an alloying process. Although some negative results have been obtained with addition of Cr or Mn, the chance of achieving positive results by adding other elements has not been excluded and will be pursued.

As a first step, we have calculated anti-phase boundary (APB) energies for two most probable APB's, namely $1/2\langle 111 \rangle$ on $\{110\}$ and $1/2\langle 111 \rangle$ on $\{112\}$. For simplicity, we introduced APB's only on $\{110\}$ or $\{112\}$ plane. Thus, the smallest supercell which maintains crystal translational symmetry has 8 atoms per unit cell, and yields an orthorhombic cell for $1/2\langle 111 \rangle \{110\}$ and a monoclinic cell for $1/2\langle 111 \rangle \{112\}$, respectively. The different nearest neighbors and second nearest neighbors in the $1/2\langle 111 \rangle \{110\}$ and $1/2\langle 111 \rangle \{112\}$ APB's and in the original B2 cell makes the lattices behave differently.

For consistency, we calculated the starting B2 symmetry lattice by using three different unit cells: the original one, the orthorhombic one and the monoclinic one. The latter two have the same size as those for the APB calculations

except that no APB was introduced. The calculated results from the three different symmetry cells are exactly the same within the precision of the method; this gives us confidence in the accuracy of the APB energy calculations. By comparing the total energy for the cells with and without an APB, we found the APB energy to be 1404 erg/cm^2 for the $1/2\langle 111 \rangle \{112\}$ APB and 1134 erg/cm^2 for the $1/2\langle 111 \rangle \{110\}$ APB. These values are extremely high, especially when compared to the result we calculated for APB in Ni_3Al (cf. Sec. D above). The APB energy for $1/2\langle 111 \rangle \{112\}$ is larger than $1/2\langle 111 \rangle \{110\}$, as expected. The energy for breaking a Ni-Al bond [$1/2(E_{\text{Ni-Ni}} + E_{\text{Al-Al}})$] is found to be 16.4 mRy for $1/2\langle 111 \rangle \{112\}$ and 15.4 mRy for $1/2\langle 111 \rangle \{110\}$ (we only consider first nearest neighbors). These two numbers showed good agreement.

In the next phase, we expanded the size of the supercell so that a more realistic representation of the APB will be given. Simultaneously, the APB energies in NiTi - the so called memory metal - was studied to determine similarities and differences from those for NiAl and to ascertain the possible role of its Martensitic phase transition in determining its ductility.

The current approach for improving the ductility of NiAl is to evaluate the effects of alloying element additions. The selection of these alloying elements has been based primarily on empirical knowledge, an approach which has met with very limited success. Our specific objective is to determine the ductilizing effects of alloying elements which will be selected utilizing alloying concepts derived from first principles. Thus, the role of ternary element additions on the electronic structure, phase stability, bonding characteristics, elastic properties, anti-phase boundaries, and slip systems of NiAl will be predicted using our quantum mechanical modelling approach and will be verified (at GE) by ductility measurements on NiAl single crystal alloys. Our goal is to determine whether alloying concepts based on first principles can be used to predict mechanical behavior of intermetallic compounds, in which case this would serve as an extremely powerful tool for accelerating the development of useful intermetallic compounds. A promising proposed candidate is Li. As a first step in selecting possible ternary additions and because it may relate to the ductility of NiTi, we will study the $L1_0$ structure and to see how ternary additions can stabilize this more ductile phase (using the density of states approach described above).

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"Electronic Structure and Properties of Cubic ZrAl_3 ", T.J. Watson-Yang, J.-H. Xu, A.J. Freeman, and T. Oguchi, (in preparation).

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"Electronic Structure of $\text{Ni}_3\text{Al}(001)$: Surface State and Antiphase Boundary (APB) Properties", A.J. Freeman, C.L. Fu, and J.I. Lee, (in preparation).

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"Electronic and Structural Properties of Metallic Li", J.J. Yu, B.I. Min, R. Podlucky, and A.J. Freeman.

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"Crystal Structure, Phase Stability and Electronic Structure of TiAl Intermetallics", T. Hong, T.J. Watson-Yang, A.J. Freeman, and T. Oguchi.

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Lectures and Seminars:

"First Principles Studies of Structural Phases Stability in the Nickel-Aluminides", Conf. on Nickel Aluminides, Wright-Patterson Air Force Base, Oct. 1985.

"Structural Stability Calculations in the Titanium-Aluminium System", Conf. on Titanium Aluminides, Wright-Patterson Air Force Base, Nov. 1986.

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"Ab Initio Calculations of Ordered Intermetallic Phase Equilibria in the Al-Li System", (with M. Sluiter, D. de Fontaine, X.Q. Guo and R. Podloucky).

"Alloy Modeling and Experimental Correlation for Ductility Enhancement in NiAl (with R. Darolia, D.F. Lahrman and R.D. Field).

"Electronic Structure and Mechanical Properties of Intermetallics: APB Energies in Ni-Al-Based Systems", (with Tao Hong).