ELECTRONIC PROPERTIES OF STOCHIOMETRIC TITANIUM - ALUMINUM CRYSTALS: I, FACE - CENTERED CUBIC TITANIUM

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الخلاصة

ان طريقة الربط الشديد المعدله التي تسمح بمعالجه متوافقه للمستويات الالكترونية في الترتيب الثنائى للسبائك قد عرضت. وقد طبقت هذه الطريقه على بلورات Ti Al₃ Ti₂ Al, Ti Al₃. سنعرض فقط في هــذا المقال طيف بلورة Fcc Ti₄. وسنراجع بعض الكميات الطبيعيه التي يمكن أن تحسب من قيم وعلاقات أيجن التي تنتج من تطبيق هذه الطريقه.

ABSTRACT

A modified Tight-Binding approach that allows a fully self-consistent treatment of the electronic states in ordered binary alloys is presented. This approach is discussed for the $Ti\,Al_3$, $Ti_2\,Al_2$, and Ti_3Al crystals. In this paper we will only report on the bandstructure of the fcc Ti_4 crystal and review some of the physical quantities that can be calculated from the eigenvalues and eigenfunctions that result from the application of this approach.

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1. INTRODUCTION

In transition-metal alloys, the crystal potential in a cell depends upon the constituent atoms occupying the cell. In general, this potential is considerably different from that describing the constituents; and the extent of sd - and pd-hybridization among the atomic energy levels is expected to be strong. Attempts at understanding the alloying mechanism have resulted in several theoretical models [1]. These models have three closely-related goals: (i) to describe and classify the alloy phases in terms of composition and crystal structure; (ii) to associate structures and structural elements with the character and distribution of the electronic charge densities; and (iii) to understand the factors which determine the relative stability of the phases. The realization of these goals needs quantitative treatments involving, for various structures, a detailed knowledge of the distribution of the electronic charge both spatially and energetically. Band theory provides a framework to study some of the characteristics of the electronic charge distributors for stochiometric alloys and will be used here to study Ti_4 and the aluminides of titanium: $TiAl_3$, Ti_2Al_2 and Ti_3Al.

These alloys are of great technological importance. They have a high melting point, good oxidation resistance, high elevated-temperature creep resistance, and favorable strength-to-weight ratios. However one of their undesirable properties is that they are brittle. Since the titanium crystal does not possess this property, then a study of the effects brought about by the successive filling of the Ti d-band complex with a higher percentage of aluminum concentration would be very informative. Apart from providing valuable information on the charge distribution (spatially and energetically), such an investigation may shed light on the reasons behind brittleness.

The potentialities of the Ti-base aluminides as high temperature alloys have been discussed first by Kormilov et al.[2]. Experimental data on the brittleness of Ti_3Al has been obtained by Blackburn and Williams [3]; and Schetchman et al.[4] have explored the mechanical properties of Ti_2Al_2. Phase diagrams as a function of the relative concentrations have been constructed [5], and several of the response functions have been graphed [6]. Other experimental investigations were carried out on the mechanical properties

(using laser radiation) [7]; on the effect of temperature on nucleation and growth of the ordered Ti_3Al phase [8]; and on strain aging[9]. A major study of fracture-toughness properties with several microstructure conditions was recently reported by Lewis [10] for two titanium aluminide alloys. The above is by no means a complete survey of the existing literature [11] and is included to reflect the diversified interests in these alloys.

In the area of transition-metal compounds, the calculations which have been reported until recently were for materials in which the one component is a transition metal and the other C, N, and O[12-14]. The electronic structure of TiFe [15,16] and several of the CsCl - type structure transition metal alloys have been calculated [16]. However, theoretical studies on the ordered Ti-aluminides are lacking [11] and will be the subject of the present investigation. The approach that will be followed here is elaborated elsewhere [17] and will only be summarized.

The Tight-Binding method of Band Theory will used to obtain the solutions of the effective one-electron Hamiltonian describing the alloy crystal in a self-consistent manner. Self-consistency is achieved by an iterative procedure: a crystal potential is constructed from a superposition of overlapping neutral-atom charge densities. The local approximation is used to generate the exchange part. Energy levels and wave functions are then determined in the potential, a new total charge density is calculated and then used to initiate the iterative procedure leading to self-consistency. The manner of constructing the crystal potential is discussed in Section 2. The Hamiltonian matrix elements and self-consistency procedure are discussed in Section 3. The band-structure of Ti_4 is presented in Section 4 and in the summary some of the relevant physical quantities that will be used in studying the electronic charge distribution and in our attempt to understand the brittleness property will be reviewed.

2. CRYSTAL POTENTIAL

To initiate this section it is appropriate to discuss the crystal structure of the alloys under consideration. Each of the crystals has four atoms per unit cell, and the lattice will be described by four interpenetrating simple cubes described by the following nonelementary translations [18]:

$$\vec{T}_1 = \frac{a}{2}(0, 0, 0,) \text{ (with full cubic symmetry)}$$

$$\vec{T}_2 = \frac{a}{2}(\tfrac{1}{2}, \tfrac{1}{2}, 0)$$

$$\vec{T}_3 = \frac{a}{2}(\tfrac{1}{2}, 0, \tfrac{1}{2}) \quad \text{(tetrahedral symmetry)} \tag{1}$$

$$\vec{T}_4 = \frac{a}{2}(0, \tfrac{1}{2}, \tfrac{1}{2})$$

which mark the points about which the cubes are centered; a is the lattice constant. In TiAl$_3$, titanium atoms are situated at the corners of the cube defined by $\vec{T}_1$, and aluminum atoms are the corners of the cubes defined by $\vec{T}_2$, $\vec{T}_3$, and $\vec{T}_4$. In Ti$_3$Al the above situation is reversed. In Ti$_2$Al$_2$, the titaniums are on the cubes defined by $\vec{T}_1$ and $\vec{T}_2$ and aluminums on $\vec{T}_3$ and $\vec{T}_4$. The remaining two cases of interest are face-centered-cubic (fcc) Ti and (fcc) Al. The band-structure of (fcc) Al has been studied earlier [17] and that of Ti will be presented in a subsequent section.

The crystal potential is constructed from a super-position of spherically averaged neutral-atom charge densities; that is

$$V(\vec{r}) = \sum_{\mu}\sum_{i=1}^{4} v_i(\vec{r} - \vec{R}_{\mu} - \vec{T}_i), \tag{2}$$

with the index i denoting the species type. $\vec{T}_i$ is defined in Equation (1), and the $\vec{R}_{\mu}$ are direct lattice vectors of the simple cubic (sc) lattice.

Since the potential is translationally invariant under the set $\{\vec{R}_{\mu}\}$, then an alternate representation is

$$V(\vec{r}) = \sum_s \exp(+i\vec{K}_s \cdot \vec{r}) \, V(\vec{K}_s), \tag{3}$$

where the $\vec{K}_s$ are reciprocal lattice vectors of the sc lattice.

Alternatively,

$$V(\vec{K}_s) = \frac{1}{N\Omega_o} \int_{\text{all space}} \exp(-i\vec{K}_s \cdot \vec{r}) \, V(\vec{r}) \, d^3r$$

$$= \frac{1}{\Omega_o} \int_{\text{unit cell}} \exp(-i\vec{K}_s \cdot \vec{r}) \, V(\vec{r}) \, d^3r \tag{4}$$

where N is the total number of sites in the crystal

and Ω_o is the volume of the Wigner-Seitz cell, or,

$$V(\vec{K}_s) = \sum_{i=1}^{4} I(\vec{K}_s, \vec{T}_i) \exp(-\vec{K}_s \cdot \vec{T}_i), \tag{5}$$

with

$$I(\vec{K}_s, \vec{T}_i) = \frac{1}{\Omega_o} \int_{\substack{\text{atomic} \\ \text{volume}}} \exp(-i\vec{K}_s \cdot \vec{r}) \, V_i(\vec{r}) \, d^3r. \tag{6}$$

Noting that $\exp(-i\vec{K}_s \cdot \vec{T}_i) = \pm 1$ and that $V_i(\vec{r})$ is constructed to be spherically symmetric (for the initial iteration) then the Fourier coefficients are only a function of the modulus of $\vec{K}_s$ i.e. $V(\vec{K}_s) = V(|\vec{K}_s|)$.

The Coulomb Potential

Recalling that in Equation 2 the Coulomb part of the potential arising from the ion of species i at site $(\vec{R}_{\mu} + \vec{T}_i)$ is

$$V_i^C(\vec{r}) = \frac{-2Z_i}{r} + 2\int_{\substack{\text{all} \\ \text{space}}} \frac{\rho_i(\vec{r}')}{|\vec{r} - \vec{r}'|} \, d^3r' . \tag{7}$$

This is in atomic units (h = 1, $e^2 = 2$, m = $\tfrac{1}{2}$) with Z_i as the nuclear charge and $\rho_i(r)$ is the electronic charge density.

Now, $V_i^C(\vec{K}_s) =$

$$\frac{1}{N\Omega_o} \sum_{\mu}\sum_{i=1}^{4} \int_{\substack{\text{all} \\ \text{space}}} \exp(-i\vec{K}_s \cdot \vec{r}) V_i^C(\vec{r} - \vec{R}_{\mu} - \vec{T}_i) d^3r$$

$$= \frac{1}{\Omega_o} \sum_{i=1}^{4} \exp(-i\vec{K}_s \cdot \vec{T}_i) \int_{\substack{\text{all} \\ \text{space}}} \exp(-i\vec{K}_s \cdot \vec{r}) V_i^C(\vec{r}) d^3r .$$

Assuming that $\rho_i(\vec{r})$ is spherically symmetric, then

$$V_i^C(\vec{K}_s) = \frac{-8\pi}{\Omega_o K_s^2} \sum_{i=1}^{4} \exp(-i\vec{K}_s \cdot \vec{T}_i) \left[Z_i - \frac{4\pi}{K_s} \right.$$
$$\left. \int_0^{\infty} r\rho_i(r) \sin(K_s r) dr \right]; \text{ for } K_s \neq 0$$

$$= -\frac{16\pi^2}{3\Omega_o} \sum_{i=1} \int r^4 \rho_i(r) d^3r \text{ for } K_s = 0. \tag{8}$$

The Exchange Potential

$$V_x(\vec{K}_s) = \frac{1}{N\Omega_o} \int_{\substack{\text{all} \\ \text{space}}} \exp(-i\vec{K}_s \cdot \vec{r}) V_x(\vec{r}) d^3r \tag{9}$$

$$= \frac{1}{\Omega_o} \int_{\text{cell}} \exp(-i\vec{K}_s \cdot \vec{r}) V_x(\vec{r}) d^3r$$

$$= \frac{1}{\Omega_o} \sum_{i=1}^{4} \exp(-i\vec{K}_s.\vec{T}_i) \int_{\substack{\text{atomic} \\ \text{volume}}} \exp(-i\vec{K}_s.\vec{r}) V_x(\vec{r}+\vec{T}_i) d^3r.$$

In the Slater approximation:

$$V_x(\vec{r}) = -3\alpha \left(\frac{3}{\pi}\right)^{1/3} [\rho_{\text{Total}} (\vec{r}+\vec{T}_i)]^{1/3}, \quad (10)$$

α is the only adjustable parameter in the theory, and ρ_{Total} is the total electron charge density in the cell.

Then,

$$V_x(\vec{K}_s) = -3\alpha \left(\frac{3}{\pi}\right)^{1/3} \sum_{i=1}^{4} \exp(-\vec{K}_s.\vec{T}_i)$$

$$\int_{\substack{\text{atomic} \\ \text{volume}}} \exp(-\vec{K}_s.\vec{r})\rho_{\text{Total}}^{1/3}(\vec{r}+\vec{T}_i) d^3r,$$

and, in terms of the angularly averaged density $\rho_A(r)$

$$V_x(K_s) = -\frac{9\alpha}{4K_s R^2_{\text{WS}}} \left(\frac{3}{\pi}\right)^{1/3} *$$

$$\sum_{i=1}^{4} \exp(-i\vec{K}_s.\vec{T}_i) \int^{R_{\text{WS}}} \rho_A^{1/3}(|\vec{r}+\vec{T}_i|(r\sin(K_s r)dr, (11)$$

where R_{WS} is the Wigner-Seitz radius defined by

$$a^3 = 4 \left(\frac{4}{3}\pi R_{\text{WS}}^3\right) \quad (12)$$

the factor of 4 is due to the number of atoms per cell.

The Crystal Field

In a cubic crystal each lattice point has twelve nearest neighbors. Suppose charges $Z_1 e$ are located at the four points given by:

$$(\pm\tfrac{1}{2}, \pm\tfrac{1}{2}, 0) a$$

and charges $Z_2 e$ are located at the eight points given by

$$(\pm\tfrac{1}{2}, 0, \pm\tfrac{1}{2}) a$$

$$(0, \pm\tfrac{1}{2}, \pm\tfrac{1}{2}) a$$

Then at a point (x, y, z) in the vicinity of the atom located at the origin, the contribution to the crystal field potential (VCF) due to the charge $Z_1 e$ at the point $a (\tfrac{1}{2}, \tfrac{1}{2}, 0)$ is

$$V_1(x,y,z) = \frac{\sqrt{2}eZ_1}{a} \left[1 + \frac{2(x+y)}{a} + \frac{2r^2}{a^2}\right]^{-\frac{1}{2}} \quad (13)$$

and for small $r = (x^2+y^2+z^2)^{\frac{1}{2}}$, the Binomial expansion to 4th order gives:

$$V_1(x,y,z) = \frac{\sqrt{2}Z_1 e}{a} \left[1 - \frac{x+y}{a} - \frac{r^2}{a^2} + \frac{3}{2}\frac{x^2+2xy+y^2}{a^2}\right.$$

$$+ \frac{3r^4}{2a^4} + \frac{3(x+y)r^2}{a^3} - \frac{5}{2}\frac{x^3}{a^3} + \frac{3x^2y+3xy^2+y^3}{a^3}$$

$$- \frac{15}{2}(x^2+2xy+y^2)r^2$$

$$\left. + \frac{35}{8}x^4 + \frac{4x^3y + 6x^2y^2 + 4xy^3 y^4 + \cdots}{a^4}\right] \quad (14)$$

Similarly, the appropriate expressions for the twelve point charges may be obtained and added to give the total crystal field potential. To the fourth order in the expansion,

$$V_{CF} = \frac{4\sqrt{2}e}{a} \left[(2Z_2 + Z_1) + \left(\frac{17}{4}Z_2 - \frac{13}{8}Z_1\right)\frac{r^4}{a^4}\right.$$

$$- \frac{35}{8}\frac{Z_2(2z^4+x^4+y^4) - Z_1 z^4}{a^4}$$

$$\left. + -\frac{1}{2}\frac{r^2}{a^2} + \frac{3}{2}\frac{z^2}{a^2} + \frac{5}{4}\frac{r^2z^2}{a^4} - \frac{35}{2}\frac{x^2y^2}{a^4}\right]. \quad (15)$$

If Z_2 is the Ti nuclear charge and Z_1 is that of Al, then Expression 15 determines the crystal field potential of the Ti_2Al_2 crystal. It is interesting to note here that this will affect the degeneracy of the p-like bands. The reason is that now there exists only one axis of rotation and the p_x and p_y symmetries will be degenerate and that of the p_z will be split. Another way of describing the situation is that the planes defined by $R_\mu = a(0,0,n)$ (n=integer, dominant for n=1) are occupied by Ti only, by and all other planes have a Ti with at least four Al atoms as nearest neighbors.

In the case of $Z_1 = Z_2 =$ nuclear charge on Ti(Al) Expression 15 determines the crystal field potential for the Ti_3Al ($TiAl_3$) crystal and the full cubic symmetry is restored (each site has 12 nearest neighbors of the same species).

In the next section, the basis functions used to construct the Block states are described, expressions for the Hamiltonian matrix are presented, and the self-consistency procedure is outlined.

3. DETAILS OF THE CALCULATION

In the Tight-Binding formulation, the Bloch basis set functions are expressable as:

$$\phi_i(\vec{k},\vec{r}) = \frac{1}{N^{\frac{1}{2}}} \sum_\mu \exp\{+i\vec{k}.(\vec{R}_\mu+\vec{T}_j\} U_i^j(\vec{r}-\vec{R}_\mu-\vec{T}_j), \quad (16)$$

for the jth species, and by

$$|\Phi_i(\vec{k},\vec{r})\rangle = \frac{1}{N^{\frac{1}{2}}}\begin{bmatrix}\phi_i^1(\vec{k},\vec{r})\\\phi_i^2(\vec{k},\vec{r})\\\vdots\quad\vdots\quad\vdots\\\vdots\quad\vdots\quad\vdots\\\phi_i^\beta(\vec{k},\vec{r})\end{bmatrix} \quad (17)$$

for a crystal with β distinct species. N is the number of sites in the crystal for a given species, $\vec{k}$ is the Bloch electron wave number, and $\vec{R}_\mu + \vec{T}_j$ defines the position

of the jth atom in the cell defined by $\vec{R}_\mu$ about which

the set of function U are localized.

The U's are taken to be a set of Gaussian-Type Orbitals (GTO)* and determined variationally in a separate Hartree-Fock calculation on the isolated atom reported by Wachter [19]. To calculate the bandstructure of the Ti_4 crystal, the localized basis set consisted of 13 orbitals for the s-symmetry, 10 for the p-symmetry and 5 for the d-symmetry. Such a basis set will yield matrices of dimensionality 68 for each of the $\vec{k}$ points. For the alloy problem, the basis will be contracted according to the groupings of contraction Number 3 of [19].

In terms of Equation 17, the wavefunction of an electron in the crystal with wavenumber $\vec{k}$ and in band n may be schematically represented as:

$$|\psi_n(\vec{k},\vec{r})\rangle = \sum_i A_{ni}(\vec{k})|\Phi_i(\vec{k},\vec{r})\rangle$$

$$= \frac{1}{N^{\frac{1}{2}}}\sum_i\begin{bmatrix}a_{ni}^1(\vec{k})\phi_i^1(\vec{k},\vec{r})\\a_{ni}^2(\vec{k})\phi_i^2(\vec{k},\vec{r})\\a_{ni}^\beta(\vec{k})\phi_i^\beta(\vec{k},\vec{r})\end{bmatrix} \quad (18)$$

The energy bands and corresponding wavefunctions for the electrons in the crystal are obtained by solving:

$$\mathcal{H}|\psi_n(\vec{k},\vec{r})\rangle = E_n(\vec{k})|\psi_k(\vec{k},\vec{r})\rangle ., \quad (19)$$

where $\mathcal{H}$ is the effective one-electron Hamiltonian given by (in atomic units)

$$\mathcal{H} = -\nabla^2 + V(\vec{r}).$$

$-\nabla^2$ is the kinetic energy term and $V(\vec{r})$ is the crystal potential discussed in Section 2.

In the space spanned by the $\phi_i^j(\vec{k},\vec{r})$ Equation 15, the secular determinant for the A_{ni} coefficients takes the form:

$$\sum_i\left\{\begin{bmatrix}H_{ni}^{11}(\vec{k}) & H_{ni}^{12}(\vec{k})\dots\\H_{ni}^{21}(\vec{k})\\\vdots\\\vdots\\H_{ni}^{\beta 1}(\vec{k}) & \dots\end{bmatrix}\right.$$

$$\left.-E_n(\vec{k})\begin{bmatrix}S_{ni}^{11}(\vec{k})\dots\\\vdots\\\vdots\\S_{ni}^{\beta 1}(\vec{k}). & \dots\end{bmatrix}\right\}\begin{bmatrix}a_{ni}^1(\vec{k})\\\vdots\\\vdots\\a_{ni}^\beta(\vec{k})\end{bmatrix} = 0 \quad (20)$$

with

$$H_{ni}^{1t} = \int \phi_n^{1*}(\vec{k},\vec{r})\,\mathcal{H}\,\phi_i^t(\vec{k},\vec{r})\,d^3r, \quad (21)$$
$$= T_{ni}^{1t} + V_{ni}^{1t}$$

and

$$S_{ni}^{1t} = \int \phi_n^{1*}(\vec{k},\vec{r})\phi_i^t(\vec{k},\vec{r})\,d^3r, \quad (22)$$

with T_{ni} as the kinetic energy matrix between the nth and jth basis functions for the species 1 and t, and correspondingly V_{ni} and S_{ni} are the crystal potential and overlap matrix elements.

In terms of the GTO,

$$T_{ni}^{1t} = \{-i\vec{k}.(\vec{T}_1-\vec{T}_t)\}\sum_\mu -i\vec{k}.\vec{R}_\mu)\int U_n^{1*}(\vec{r})(-\nabla^2)$$
$$U_i^t(\vec{r}-\vec{R}_\mu+\vec{T}_1-\vec{T}_t)\,d^3r, \quad (23)$$

$$V_{ni}^{1t} = \exp\{-i\vec{k}.(\vec{T}_1-\vec{T}_t)\}\sum_{\mu,K_s}\exp(-i\vec{k}.\vec{R}_p)V(\vec{K}_s)$$

$$\int U_n^{1*}(\vec{r})\exp(-i\vec{K}_s.\vec{r})U_i^t(\vec{r}-\vec{R}_\mu+\vec{T}_1-\vec{T}_t)d^3r, \quad (24)$$

and,

$$S_{ni}^{lt} = \exp\{-i\vec{k}.(\vec{T_1}-\vec{T_t})\} \sum_{\mu,K_s} \exp(-i\vec{k}.\vec{R}_\mu) \int U_n^{l*}(\vec{r})$$

$$U_i^t (\vec{r}-\vec{R}_\mu+\vec{T_1}-\vec{T_t}) \, d^3r \qquad (25)$$

Explicit expressions for Equations 23-25 may be obtained directly from the authors.

Diagonalizing the secular determinant (Equation 2) yields the energy eigenvalues, and the corresponding wavefunctions by determining the $A_{ni}(\vec{k})$ coefficients in Equation 18. Using this expression for the electronic Bloch states and noting that the charge density $\rho(\vec{r})$ has the crystal periodicity, the Fourier coefficients of the charge density $\rho(\vec{K_s})$ are calculated from the following expression

$$\rho(K_s) = \sum_{i,k} A^*_{ni}(\vec{k})A_{nj}(\vec{k}\ \langle\phi_i(\vec{k},\vec{r})|\exp(i\vec{K_s}.\vec{r})|\phi_j(\vec{k},\vec{r})\rangle$$

$$(26)$$

where the $\vec{k}$ summation is carried out for occupied states. Since only the Fourier coefficients of the potential are required in this formalism, the new $V(\vec{K_s})$ used to initiate the self-consistency procedure are related to the $\rho(\vec{K_s})$ by

$$V(\vec{K_s}) = -8\pi \rho(\vec{K_s}) / \vec{K_s}^2. \qquad (27)$$

A new Hamiltonian is obtained by using the new set of $V(\vec{K_s})$ in Expression 24, and the self-consistency procedure is terminated when $\Delta\rho(\vec{K_s})/\rho(\vec{K_s})<10^{-5}$. $\Delta\rho(\vec{K_s})$ is the difference between two consecutive iterations. In this procedure it was not necessary to spherically average the charge density. Only the first 19 coefficients were changed. The effect of self-consistency on the $V(\vec{K_s})$ is displayed in Table 1.

The above outlined procedure is applied to obtain the handstructure of the Ti_4 fcc crystal and the results obtained are reported in the next section.

4. BANDSTRUCTURE OF fcc Ti₄

The calculation of the bandstructure of fcc titanium was begun by constructing a crystal potential from a superposition of overlapping neutral-atom charge densities, the atoms assumed to be in the $3d^3 4s^1$ configuration. The wavefunctions used in forming this atomic charge density were taken from the Hartree-Fock self-consistent-field calculations of Clementi [20], which are linear combinations of Slater-type orbitals. Contributions from the first 12 shells of neighbors ensured convergence of the Hamil-

tonian matrix elements in the direct lattice summation while the $\vec{K_s}$ summation was carried to 20000 unique vectors in order to achieve convergence. Energy levels and wavefunctions were determined for this potential and used to initiate the self-consistency procedure. In this process the first 20 Fourier coefficients of the potential were corrected using the wavefunctions of the occupied states at 43 points in 1/48th of the Brillouin zone. Table 1 displays the $V(\vec{K_s})$ coefficients and the accompanied changes due to self-consistency. The exchange parameter was set equal to 2/3.

Table 1. Some Fourier Coefficients of the Crystal Potential. The Smallest 19 Reciprocal-lattice Vectors are Listed. The Change in These Quantities Resulting from the Iterative Process is Given.

$\vec{K_s}$	$Vc(\vec{K_s})$	$\Delta Vc(\vec{K_s})$	$V_x(\vec{K_s})$	$\Delta V_x(\vec{K_s})$
111	−1.7678	−0.0485	−0.2047	+0.0221
200	−1.2398	−0.0421	−0.1036	+0.0332
220	−0.5007	−0.0046	−0.0237	+0.0091
311	−0.3228	+0.0007	−0.0429	−0.0098
222	−0.2859	+0.0020	−0.0457	−0.0123
400	−0.1912	+0.0020	−0.0338	−0.0092
331	−0.1505	+0.0021	−0.0146	−0.0017
420	−0.1403	+0.0019	−0.0088	+0.0005
422	−0.1093	+0.0018	+0.0047	+0.0051
333	−0.0933	+0.0016	+0.0045	+0.0043
511	−0.0933	+0.0015	+0.0045	+0.0043
440	−0.0745	+0.0013	−0.0060	−0.0007
531	−0.0662	+0.0012	−0.0123	−0.0033
442	−0.0638	+0.0011	−0.0138	−0.0039
600	−0.0638	+0.0010	−0.0138	−0.0039
620	−0.0556	+0.0009	−0.0163	−0.0047
533	−0.0506	+0.0009	−0.0147	−0.0037
622	−0.0491	+0.0008	−0.0136	−0.0031
444	−0.0439	+0.0008	−0.0083	−0.0005

Table 2. Some Energy Differences at High Symmetry Points (Rydbergs.)

$\Gamma'_{25} - \Gamma_1$	0.9088	$X_3 - X_1$	0.1303
$\Gamma_{12} - \Gamma_1$	1.1220	$X'_4 - X_1$	0.2396
$L'_2 - L_1$	0.2916	$X_5 - X_1$	0.7839
$L_3 - L_1$	0.5041	$X'_5 - X_1$	0.9755
$W_3 - W'_2$	0.0868	$K_3 - K_1$	0.3191
$W_1 - W'_2$	0.3266	$K_4 - K_1$	0.5930
$W'_1 - W'_2$	0.6895	$K_2 - K_1$	0.6983

d−bandwidth = 0.8156 Rydbergs

Fermi energy = 0.0853 Rydbergs

The calculated bandstructure is shown in Figure 1 for several symmetry directions, and Table 2 displays some of the more energy differences. The lattice constant is taken to be 4.1330 A.

A direct comparison with the results of other calculations is not possible because these treated the hcp[21,22] and bcc[23] phases for this metal. However, this calculation is valuable as it stands because it will be used as the reference for studying the titanium-aluminum alloying process.

5. SUMMARY

In this paper, an account of a fully self-consistent scheme to obtain the solutions of the effective one-electron Hamiltonian of some stochiometric binary alloys is presented and applied to obtain the bandstructure of fcc titanium. The self-consistent wavefunctions and corresponding energy spectrum can be readily used to calculate several experimentally measurable quantities.

The eigenvalues can be used to calculate the total electronic density of states and to investigate the Fermi surface topology. Contributions to the density of states from each of the parent atoms can be isolated; and this can be further decomposed into its sp-and d-symmetry components. The information thus obtained can be used to investigate the applicability of the rigid band model. The susceptibility, $\chi(q)$ can be calculated and its structure can be related to electronically induced instabilities [24].

The wavefunctions, on the other hand, can be used to study the x-ray form factors and the Compton profiles. Respectively, this study will provide information on the localized and diffuse nature of the electronic charge distribution. Also, charge density maps can be constructed and will be used to study charge transfers accompanying the alloying process. The anisotropy in the charge distribution can be used to study the bonding effects, and an attempt will be made to relate this to the existence of sheer and slip planes of the system.
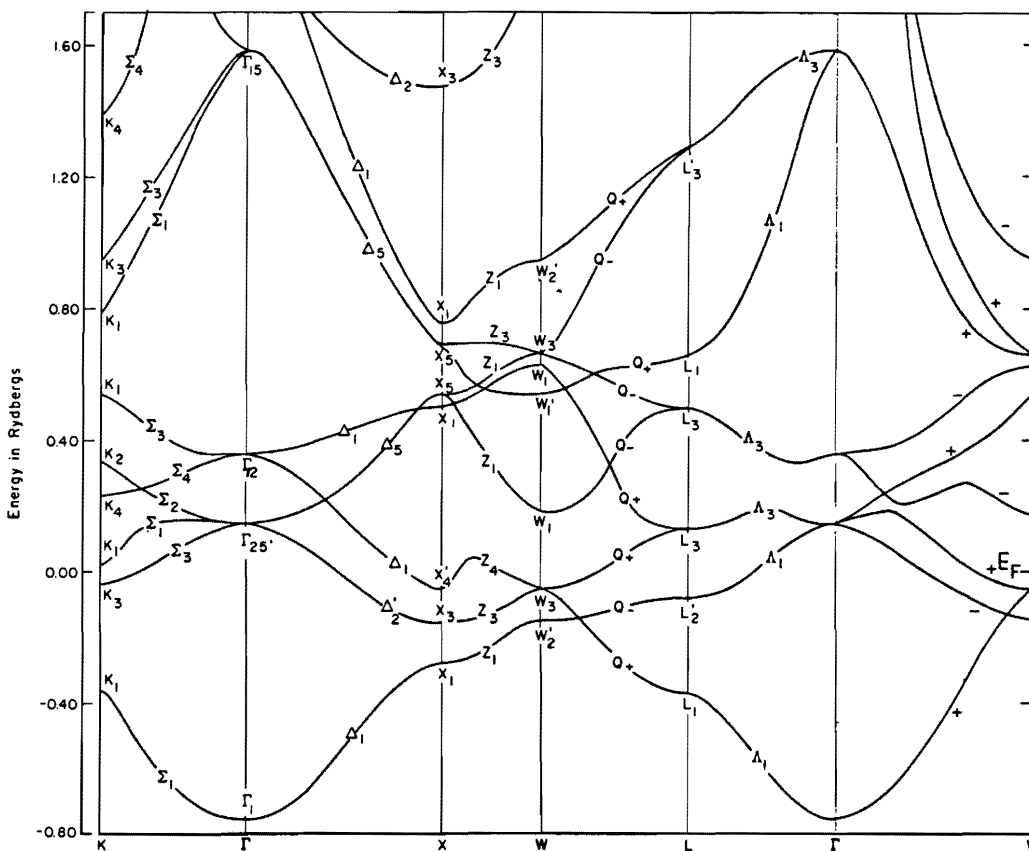

FIGURE. I. BANDSTRUCTURE OF FCC Ti

These physical quantities are being studied presently for the aluminides of titanium mentioned in this paper, and will be reported upon in future communications.

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