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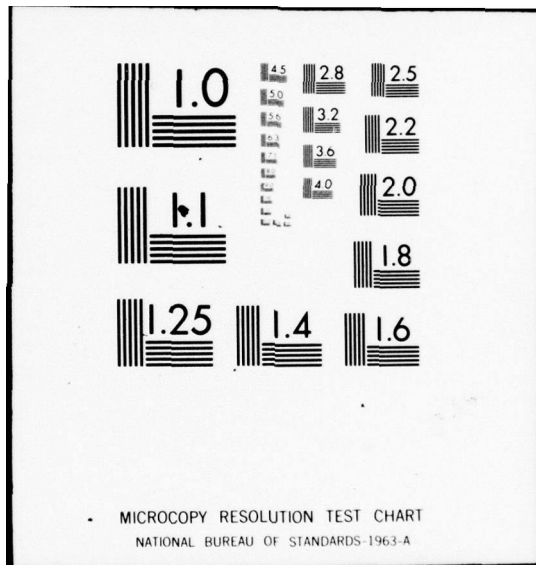
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November 1977

INTERFACE ENERGIES

Cheng-Chih Pei

Department of Physics, University of California San Diego
La Jolla, California 92093

Abstract

We developed a practical scheme for the calculation of interface energies. It combines the theory of generalized Wannier functions, the generalized recursion method for calculating local densities of states and electronic density, and the local density functional theory. As a first application of this method we are calculating the stacking fault energy of nickel using tight binding type Wannier functions for the d-electrons and ignoring the effect of the s-electrons. The d band degeneracy is fully taken into account. The method also allows one to handle charge transfer effects: a stacking fault perturbation potential is included and calculated quasi-self-consistently. Comparison is made between the moment scheme, the non-self-consistent scheme and the self-consistent scheme. We find that the self-consistent scheme affects very little the stacking fault energy compared with the non-self-consistent scheme.

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Chapter I

Introduction

Hohenberg and Kohn¹ and Kohn and Sham² (KS) developed a procedure for determining the ground state energy of a system of interacting electrons subject to an external potential. This procedure involves the solution of a single particle Schrödinger equation for an electron moving in an effective potential that is determined self-consistently. Traditional methods of solving this one-particle Schrödinger equation for crystalline solids have involved obtaining the Bloch band structure. A perfect infinite and periodic lattice is an essential ingredient in this method. If one is to deal with non-periodic solids, such as clean or overlayered solid surfaces, interfaces, problems associated with bulk impurities, stacking faults, vacancies, etc. the eigenstates and eigenvalues of this Schrödinger equation are very difficult or impossible to solve for. In addition to this difficulty of calculating the eigenstates and eigenvalues, the iterative procedure described by KS is in general quite time-consuming to implement as has been pointed out several times.³ In this part, we want to develop a practical scheme for the calculation of the ground state energy for transition metals in a non-periodic system.

Because of the localized nature of the d orbitals, it seems reasonable to study the role of the d -electrons in the properties of transition metals in the tight binding approximation. A recursion

method to calculate approximately the local electron density of states and charge density within the tight binding model developed by Haydock et al.⁴ and Rehr and Pei⁵ in a non-periodic system without the necessity of calculation eigenstates of the one-particle Schrödinger equation.

We now discuss our procedure for handling the iterative difficulty. The KS self-consistency loop goes as follows:

Starting from a trial electron density $n^0(r)$, one constructs the effective potential and finds a new $n(r)$. A new effective potential is then generated and the entire procedure is iterated until self-consistency is reached.

Since the ground state energy has the stationary property with respect to $n(r)$, the error of the ground state energy is of the second order in the error of $n(r)$. That means even without any iteration, we still can have very accurate results of the ground state energy provided we choose a good initial trial $n^0(r)$. Again, because of the localized nature of the d orbitals, the state of the electron in a crystal is very similar to that in the free atom. Therefore, a superposition of partially overlapping charge densities for individual atoms placed on the appropriate lattice sites will be a very natural and good choice for the initial trial $n^0(r)$.

A description of our method for calculating the ground state energy is presented in Chapter II. In Chapter III, we present a

simple illustration of this method in which the stacking fault energy is calculated for a nickel in the $3d^{10}4s^0$ configuration. In Chapter IV, we study the stacking fault energy for a nickel crystal in the $3d^{9.4}4s^{0.6}$ configuration with a self-consistent method. Finally, Chapter V contains a discussion and a comparison with some related methods.

Chapter II

Calculational Procedure

The general scheme of our method is indicated by the "flow chart" of Fig. 1. A more detailed discussion of this flow chart is given in the following paragraphs.

The ground state atomic wave functions are taken from the Herman and Skillman atomic orbitals.⁶ These functions are fitted by a set of Gaussians in order to facilitate the subsequent Hamiltonian matrix element computations. The atomic charge densities of electrons, described by these atomic wave functions, are chosen to be spherically symmetric and the total electronic charge density in the crystal is constructed by adding the overlapping charge distributions produced by neutral atoms placed on the appropriate lattice sites.

From this electron charge density the effective potential is constructed. An important saving in computation time is obtained by separating the effective potential $V_{\text{eff}}(r)$ into a sum of overlapping spherically symmetric atomic effective potential $V_{\text{eff}}^a(r)$ plus a corresponding correction term $\Delta V_{\text{eff}}(r)$ (this term comes from the nonlinearity of the exchange and correlation potential):

$$V_{\text{eff}}(r) = \sum_{\underline{k}} V_{\text{eff}}^a(r - \underline{k}) + \Delta V_{\text{eff}}(r) \quad , \quad (2.1)$$

where

$$V_{\text{eff}}^a(\underline{r}) = \frac{Z}{|\underline{r}|} + \int \frac{n^a(\underline{r}')}{|\underline{r} - \underline{r}'|} d\underline{r}' + \mu_{xc}(n^a(\underline{r})) \quad (2.2)$$

$$\Delta V_{\text{eff}}(\underline{r}) = \mu_{xc}(n^0(\underline{r})) - \sum_{\underline{l}} \mu_{xc}(n^a(\underline{r} - \underline{l})) \quad (2.3)$$

$$n^0(\underline{r}) = \sum_{\underline{l}} n^a(\underline{r} - \underline{l}) \quad (2.4)$$

Here \underline{l} runs over all the lattice sites, and

$$\mu_{xc}(n(\underline{r})) = d(\mathcal{N} \epsilon_{xc}(n)) / d\mathcal{N} \quad (2.5)$$

where $\epsilon_{xc}(n)$ is the exchange and correlation energy per electron of a uniform gas of density \mathcal{N} . The first and second terms on the right hand side of Eq. (2.2) are the Coulomb potential and the third term is the exchange and correlation contribution to the chemical potential of a uniform gas of density \mathcal{N} . Again, for facilitating the subsequent Hamiltonian matrix elements computation, the atomic effective potential is fitted to the following "Gaussian" form:

$$V_{\text{eff}}^a(\underline{r}) = \frac{c_1 e^{-d_1 r^2}}{|\underline{r}|} + \sum_{i=2}^M c_i e^{-d_i r^2} \quad (2.6)$$

$\Delta V_{\text{eff}}(\underline{r})$, the nonlinear part of the exchange and correlation potential is small and a weak function of \underline{r} , which in the first order approximation, can be treated as a constant $\langle \Delta V_{\text{eff}}(\underline{r}) \rangle$. This

constant can be obtained by taking an average of the values of $\Delta V_{\text{eff}}(r)$ over a unit cell.

At the same time, the generalized Wannier functions⁷ (GWF) of d orbitals are constructed from these normalized atomic orbitals. These GWF $a_{\underline{l}}^{\alpha}(r)$ are localized respectively about the lattice sites \underline{l} and orthogonalized by the Löwdin algorithm⁸ with respect to all the orbitals (including $1s$, $2s$, $2p$, $3s$, $3p$, and $3d$ orbitals) which are localized at the nearest neighbors of \underline{l} .

If we choose these orthonormal GWF as localized basis functions, we can calculate the matrix elements of the Hamiltonian H for various relative orientation of sites (see Appendix A). In our computations only the nearest neighbor interaction have been included. In this case, the matrix elements of H can be expressed in terms of the self energies and the nearest neighbor hopping integrals.

Several techniques^{4, 9, 10, 11} have been developed to calculate the local electronic density of states from the matrix elements of a tight binding Hamiltonian in a non-periodic system. In the following we shall use a relatively new and powerful generalized recursion method which was developed by Haydock et al.⁴ and generalized by Rehr and Pei⁵ to find the local electronic density of states $\eta_{\underline{l}}(E)$ and the electron charge density $n(\underline{r})$.

Before proceeding with the calculations of $\eta_{\underline{l}}(E)$ and $n(\underline{r})$, let us briefly review the basic structure of the recursion method.

In this method the local density of states at a given site, say at site \underline{l} , is calculated from the diagonal Green's function matrix element:

$$\eta_{\underline{l}}(E) = \sum_{\alpha} \eta_{\underline{l}}^{\alpha}(E) \quad (2.7)$$

$$\eta_{\underline{l}}^{\alpha}(E) = \lim_{\varepsilon \rightarrow 0} -\frac{1}{\pi} \text{Im} G_{\underline{l}\underline{l}}^{\alpha\alpha}(E+i\varepsilon) \quad , \quad (2.8)$$

where α is the index describing the type of the corresponding orbital at site \underline{l} (for a 5-fold d band, there are five types of orbitals at each lattice site), and where $G_{\underline{l}\underline{l}}^{\alpha\alpha}(E)$ is evaluated using a continued fraction representation:

$$\begin{aligned} G_{\underline{l}\underline{l}}^{\alpha\alpha}(E) &\equiv \langle \alpha, \underline{l} | (E-H)^{-1} | \alpha, \underline{l} \rangle \\ &= \frac{1}{E - a_{\underline{l},0}^{\alpha} - \frac{b_{\underline{l},0}^{\alpha}}{E - a_{\underline{l},1}^{\alpha} - \frac{b_{\underline{l},1}^{\alpha}}{\dots}}} \end{aligned} \quad (2.9)$$

Here $|\alpha, \underline{l}\rangle$ denotes a GWF of type α at site \underline{l} . For the moment we restrict our discussion to a particular α , for simplifying the notation the explicit α dependence will be suppressed.

The coefficients $a_{\underline{l},j}$ and $b_{\underline{l},j}$ in Eq. (2.9) are precisely the coefficients of a 3-term recursion relation, which defines a new basis $|\underline{l}, j\rangle$ in which the Hamiltonian has a "tridiagonal" representation (a tridiagonal matrix is one whose non-zero elements

appear only on the main diagonal and the two sub-diagonals, upper right and lower left):

$$|\underline{l}, -1\rangle = 0 \quad , \quad |\underline{l}, 0\rangle = |\underline{l}\rangle$$

$$|\underline{l}, j+1\rangle = (H - a_{\underline{l}, j})|\underline{l}, j\rangle - b_{\underline{l}, j-1}|\underline{l}, j-1\rangle \quad (2.10)$$

where

$$a_{\underline{l}, j} = \frac{\langle \underline{l}, j | H | \underline{l}, j \rangle}{\langle \underline{l}, j | \underline{l}, j \rangle} \quad ; \quad b_{\underline{l}, j} = \frac{|\langle \underline{l}, j | H | \underline{l}, j+1 \rangle|^2}{\langle \underline{l}, j | \underline{l}, j \rangle \langle \underline{l}, j+1 | \underline{l}, j+1 \rangle} \quad (2.11)$$

We shall refer to the states $|\underline{l}, j\rangle$ in this semi-infinite, one-dimensional basis as "shell states," j being a shell index, since, roughly speaking, they are spatially localized about the j th shell of neighbors surrounding the atom at site \underline{l} .

Following the generalized recursion method,⁵ we can write the single particle energy ϵ and the electron charge density $n(\underline{l})$:

$$\epsilon = \sum_{\underline{l}} \int^{E_F} E n_{\underline{l}}(E) dE \quad (2.12)$$

where the Fermi energy E_F is fixed by the condition

$$N = \sum_{\underline{l}} \int^{E_F} n_{\underline{l}}(E) dE \quad (2.13)$$

N being the total number of electrons in the system and

$$n(\underline{r}) = \sum_{\underline{l}, j} a_{\underline{l}, j}(\underline{r}) A_{\underline{l}, j}(\underline{r}) \int_0^{E_F} P_{\underline{l}, j}(E) \eta_{\underline{l}}(E) dE \quad (2.14)$$

where $A_{\underline{l}, j}(\underline{r})$, the normalized shell states, can be expressed as linear combination of GWF:

$$A_{\underline{l}, j}(\underline{r}) = \frac{\langle \underline{r} | \underline{l}, j \rangle}{\{ \underline{l}, j | \underline{l}, j \}^{1/2}} \quad (2.15)$$

and where $P_{\underline{l}, j}(E)$ are the orthonormalized polynomials which are generated by a recursion relation identical to the one obeyed by the shell states. This ortho-normalization is in the following sense:

$$\int P_{\underline{l}, j}(E) P_{\underline{l}, j'}(E) \eta_{\underline{l}}(E) dE = \delta_{jj'} \quad (2.16)$$

Let us now return to the case of a composite band (such as a 5-fold d band complex), the single particle energy ϵ and the electron charge density are given, respectively, by

$$\epsilon = \sum_{\alpha} \epsilon^{\alpha} \quad (2.17)$$

$$n(\underline{r}) = \sum_{\alpha} n^{\alpha}(\underline{r}) \quad (2.18)$$

An important remark about this method should be made:

The self-consistent Hamiltonian must have the property that the total electronic charge, calculated with a unique E_F , precisely cancel the total ionic charge.

With this self-consistent ϵ and $n(r)$, we can calculate the ground state energy of the system by the KS equation:

$$E = \epsilon - \frac{1}{2} \int \frac{n(r)n(r')}{|r-r'|} dr dr' + \int n(r) [\epsilon_{xc}(n(r)) - \mu_{xc}(n(r))] dr \quad (2.19)$$

Chapter III

Example: Stacking Fault Energy of a Nickel Crystal in $3d^{10}4s^0$ Configuration

In this chapter we apply the method developed in Chapter II to the calculation of the stacking fault energy of nickel in the $3d^{10}4s^0$ configuration, the hypothetical case of filled d bands (the actual number of d electron in metallic Ni is about 9.4/atom). Before proceeding with the calculation, let us briefly review the properties of a stacking fault.

A compact structure can be described as a stacking of hexagonal close packed planes A, B and C; f. c. c. and h. c. p. lattices being respectively defined by periodic successions ABCABC and ABAB as shown in Fig. 2.

In a f. c. c. lattice, there are two types of stacking faults. The first is an intrinsic stacking fault, which is obtained by removing a plane of atoms, i. e. ABCA|CAB as shown in Fig. 2(c). The second is an extrinsic stacking fault, which is obtained by inserting an extra plane C between plane A and plane B, i. e. ABCACBCA as shown in Fig. 2(d). All the above faults preserve close packing, so that any atom keeps the same number of the nearest neighbors at the same distances. Thus, it is reasonable to assume that the formation of these faults will require a small energy. From the experimentally determined stacking fault energies γ_{SF} , they are seen to be indeed small compared to the surface energies γ_s and grain boundary

energies γ_G in f. c. c. lattices (for example, in Ni $\gamma_{SF} = 220 \text{ ergo/cm}^2$ ¹², $\gamma_S = 2000 \text{ ergo/cm}^2$ ¹³, $\gamma_G = 930 \text{ ergo/cm}^2$ ¹⁴). Although they are small energies, the stacking fault energies are very important from a metallurgical point of view, since they govern some of the plastic properties of metals and are useful for the study of the relative stability of f. c. c. and h. c. p. phases.¹⁵

Let us now return to our calculation. We want to obtain a reasonably accurate expansion for the atomic wave functions $\Psi_n(r)$ (n is the index of state, i. e. s, p, d, etc.) which are calculated by Herman and Skillman⁶ in terms of a number of Gaussian type orbitals $G_m(\alpha, r)$:

$$G_m(\alpha, r) \equiv r^{m-1} e^{-\alpha r^2} \quad (3.1)$$

where m denotes the types of the Gaussian, for example, m equals 1, 2 and 3 denote s, p and d types, respectively.

$$\Psi_n(r) \cong \sum_{i=1}^M c_i G_m(\alpha_i, r) \quad (3.2)$$

The $2M$ parameters α_i and c_i are to be chosen so as to make the approximation as good as possible. The most convenient criterion to use is to minimize a weighted squared deviation,

$$D \equiv \sum_p \left[\Psi_n(r_p) - \sum_{i=1}^M c_i G_m(\alpha_i, r_p) \right]^2 \omega(r_p) \quad (3.3)$$

where $\omega(r_p)$ is a weight function, and its choice is governed by the use to which the expansion is to be put. For example, our purpose of the expansion is to facilitate a three-dimensional integration in which r is the distance from a given center, then, in Eq. (3.3), we would choose

$$\omega(r) = r^2 \quad (3.4)$$

which is proportional to the volume of an element of spherical shell of radius r .

The selection of the best set of the exponential parameters $\{\alpha_i\}$ and the coefficients $\{c_i\}$ presents considerable difficulties. This is due to the existence of multiple minima for the value of D in the space spanned by variational parameters $\{\alpha_i, c_i\}$. Therefore, it is not claimed that we have obtained and listed true optimum values of $\{\alpha_i, c_i\}$ in table 1. The sets in table 1 are actually chosen in such a way, that they fit the function $\Psi_n(r)$ uniformly in the whole range of r .

The minimization is performed using an efficient IBM Fortran program and the "best" set of $\{\alpha_i, c_i\}$ are given in table 1.

We use the same routine to expand the atomic effective potential in terms of a number of "Gaussian" which are shown in Eq. (2.6) and the exponential parameters and the coefficients are given in table 2. The values of $\langle \Delta V_{eff}(r) \rangle$ for a perfect crystal and

a stacking fault are 0.148669087 au and 0.148669870 au, respectively.

In the case of a filled band the integral of Eq. (2.14) vanishes by Eq. (2.16), except when $j=0$. Thus the expression for $n(r)$ reduces to a trace over all the GWF:

$$n(r) = \sum_{\alpha} \sum_{\underline{l}} |a_{\underline{l}}^{\alpha}(r)|^2 \quad (3.5)$$

and the expression for ϵ reduces to a trace of Hamiltonian over all the GWF:

$$\epsilon = \sum_{\alpha} \sum_{\underline{l}} \langle \alpha, \underline{l} | H | \alpha, \underline{l} \rangle \quad (3.6)$$

where $\langle \alpha, \underline{l} | H | \alpha, \underline{l} \rangle$ is the self-energy of type α at site \underline{l} .

We shown in Appendix B that the stacking fault energy for a filled band nickel is 1.98 ergs/cm² which is very small compared to the measured stacking fault energy 220 ergs/cm². The difference between our theoretical estimate and the measured value is mainly due to the fact that our model treats Ni as a filled band metal. We note that a vanishing result was obtained by other theoretical calculations¹¹ using a full d-band.

Chapter IV

Stacking Fault Energy of Nickel in the $3d^{9.4}4s^{0.6}$ Configuration

In this chapter we apply the method explained in Chapter II to a model for paramagnetic nickel.

We know from the energy band calculations¹⁶ that there are 9.4 d electrons per atom in a solid nickel crystal. Therefore, we will calculate the stacking fault energy of solid nickel in the $3d^{9.4}4s^{0.6}$ configuration. In this calculation, we neglect the effects of sd band hybridization and study only the role of the d electrons in the stacking fault energy in the Hartree approximation. To do this calculation we follow the same procedure as we mentioned in Chapter II except for constructing the atomic effective potential $V_{eff}^a(r)$. Since the 4s wave function is highly extended in space, it is necessary to sum several shells (> 10) of neighbors in order to obtain an accurate value of $V_{eff}^a(r)$ (see Eq. (2.1)). In order to reduce computation time, we separate the atomic electronic density into what we will call a localized atomic charge density $\bar{n}^a(r)$ which receives contributions from the 1s, 2s, 2p, 3s, 3p, and 3d states and a non-localized atomic charge density $n^{a'}(r)$ which is made up from the 4s state:

$$n^a(r) = \bar{n}^a(r) + n^{a'}(r) \quad (4.1)$$

and construct $V_{eff}^a(r)$ and $\Delta V_{eff}^a(r)$ in the following fashion:

$$V_{\text{eff}}^a(\underline{r}) = \frac{Z}{|\underline{r}|} + \int \frac{n^a(\underline{r}')}{|\underline{r} - \underline{r}'|} d\underline{r}' + \mu_{xc}(\bar{n}^a(\underline{r}))$$

$$\Delta V_{\text{eff}}(\underline{r}) = \mu_{xc}(n^a(\underline{r})) - \sum_{\underline{l}} \mu_{xc}(\bar{n}^a(\underline{r} - \underline{l})) .$$

(4.2)

Here we will calculate the stacking fault energy using the following three schemes: 1. the moment scheme¹¹; 2. the non-self-consistent scheme¹⁷; and 3. the self-consistent scheme¹⁸:

1. The moment scheme

We approximate the density of states by a Gaussian multiplied by a polynomial (Edgeworth series) fitted to the four first moments (see Fig. 4):

$$n_{\underline{l}}(E) = \frac{10}{\sqrt{2\pi}\mu_2(\underline{l})} e^{-\frac{\alpha^2}{2}} \left[1 + \frac{A-3}{24} (3-6\alpha^2+\alpha^4) + \frac{B}{2} \alpha \left(-1 + \frac{\alpha^2}{3} \right) \right], \quad (4.3)$$

where

$$\alpha = \frac{E}{\sqrt{\mu_2(\underline{l})}}$$

$$A = \mu_4(\underline{l}) / \mu_2^2(\underline{l})$$

$$B = \mu_3(\underline{l}) / \mu_2^{3/2}(\underline{l}), \quad (4.4)$$

and where $\mu_2(\underline{l})$, $\mu_3(\underline{l})$ and $\mu_4(\underline{l})$ are the second, third and fourth moments of the site \underline{l} , respectively. In this scheme we use Eq. (2.13) to determine the Fermi levels E_F^{SF} and E_F^B of the crystal with and without a stacking fault. The stacking fault energy is given by

$$\begin{aligned} \Delta E &= \sum_{\underline{l}} \int_{E_F^{SF}}^{E_F^{SF}} E \eta_{\underline{l}}^{SF}(E) dE - \sum_{\underline{l}} \int_{E_F^B}^{E_F^B} E \eta_{\underline{l}}^B(E) dE \\ &= \int_{E_F^B}^{E_F^{SF}} (E - E_F^B) \left[\sum_{\underline{l}} \eta_{\underline{l}}^{SF}(E) - \sum_{\underline{l}} \eta_{\underline{l}}^B(E) \right] dE, \end{aligned} \quad (4.5)$$

where the superscripts SF and B denote the system with and without the stacking fault energy, respectively. The stacking fault energy calculated by this scheme is 18.50 ergs/cm².

2. The non-self-consistent scheme

This scheme is analogous to the moment scheme. The important feature here is the continued fraction representation; it is one of the best methods of reconstructing a density of states from a set of continued fraction coefficients (see Fig. 3(a)). This reconstructed density of states has the property of having the correct leading $2N+2$ moments if the correct leading continued fraction coefficients a_j , b_j ; $j=0, \dots, N$ are used. Using the density of state $\eta_{\underline{l}}(E)$ which is constructed by this recursion method correct to ten continued fraction coefficients and Eq. (4.5), we obtain for the stacking fault energy a value of 60.20 ergs/cm².

3. The self-consistent scheme

We know that in a metal the perturbing potential due to a stacking fault is completely screened out over a few interatomic distances. The Fermi level is the same as for the perfect crystal. However in the moment and the non-self-consistent schemes, we introduce a non-physical variation of the Fermi level for a system with a stacking fault to satisfy the charge neutrality requirement. In order to avoid this problem, we use a self-consistent scheme introduced by Allan¹⁸ to insure both that the Fermi level of a system with the stacking fault is the same as that of a perfect crystal and that charge neutrality is maintained. Since the perturbing potential is well localized near the stacking fault, the main difference between the self-consistent and non-self-consistent Hamiltonian will be its diagonal elements

$\langle \alpha, \underline{l} | H | \alpha, \underline{l} \rangle$ where \underline{l} denotes a stacking fault site. We denote this difference by u_o and adjust it so that, using the bulk Fermi level E_F^B throughout the stacking fault region is electrically neutral:

$$\sum_{\underline{l}} \int_{E_F^B}^{E_F^B} n_{\underline{l}}^{SF}(E, u_o) dE = \sum_{\underline{l}} \int_{E_F^B}^{E_F^B} n_{\underline{l}}^B(E) dE \quad (4.6)$$

In the presence of a stacking fault we know from the non-self-consistent calculation that u_o should be a very small quantity compared with the bandwidth. Therefore, we can assume in this range that the

change of total charge at the stacking fault planes is linearly proportional to the change in u_0 . Using linear interpolation instead of the truly self-consistent loop, we obtain $u_0 = 1.13 \times 10^{-4}$ a.u. .

The stacking fault energy in the self-consistent Hartree approximation is given by

$$\Delta E = \sum_{\underline{l}} \int_{E_F}^{E_F^B} E n_{\underline{l}}^{SF}(E, u_0) dE - \sum_{\underline{l}} \int_{E_F}^{E_F^B} E n_{\underline{l}}^B(E) dE - \frac{1}{2} \int [n_0(r) + \Delta n(r)] [V_0(r) + \Delta V(r)] dr + \frac{1}{2} \int n_0(r) V_0(r) dr \quad (4.7)$$

where n_0 and V_0 are the electron density and the potential in the perfect crystal. In the crystal with a stacking fault these quantities are changed into $n_0 + \Delta n$ and $V_0 + \Delta V$. The first two of Eq. (4.7) corresponds to the one-electron contribution. The last two terms of Eq. (4.7) are added to prevent the double counting of Coulomb interactions occurring in the integral. It can be written as

$$-\frac{1}{2} \left[\int n_0(r) \Delta V(r) dr + \int \Delta n(r) V_0(r) dr + \int \Delta n(r) \Delta V(r) dr \right] \quad (4.8)$$

It is easy to show that the first two terms in Eq. (4.8) give an equal contribution. Here we must notice that ΔV is well localized near the stacking fault and the preponderant term in n_0 is $j=0$ (see Eq. (2.14)). Therefore we can rewrite Eq. (4.8) under the form

$$-Z_B u_0 - \frac{1}{2} (Z_{SF} - Z_B) u_0 \quad (4.9)$$

where Z_B and Z_{SF} are the number of d-electrons per atom in the bulk and on the stacking fault, respectively. The stacking fault energy calculation by this scheme is 64.28 ergs/cm^2 .

Chapter V

Comparison and Discussion

For purposes of comparison we have drawn the bulk density of states computed with ten continued fraction coefficients (a_j, b_j ; $j = 0, \dots, 9$) and a histogram deduced from Pettifor¹⁹ with the appropriate scaling in Fig. 3(a). The good agreement of our results for the bulk density of states with band structure calculations gives us confidence in our further discussion.

We have also calculated the stacking fault energies with these three schemes which were discussed in Chapter IV using the Slater-Koster overlap parameters $dd\sigma$, $dd\pi$ and $dd\delta$ to calculate the nearest neighbor hopping integrals instead of using our constructed Hamiltonian. The parameters we have used are (in atomic units)

$$dd\sigma = -0.020838 \quad dd\pi = 0.009421 \quad dd\delta = -0.0011655$$

which was chosen by Desjonquérés *et al.*²⁰ The results of these calculations are given in Table 3.

From Table 3, we can draw the following conclusions:

1. To replace our constructed Hamiltonian by a parameterized Hamiltonian seems to have very little effect on the stacking fault energy.
2. The density of states which is correct to the fourth moment is not good enough for the stacking fault energy calculations.

3. The difference between the numerical values of the stacking fault energies obtained in the non-self-consistent scheme and that obtained in the self-consistent scheme is very small.

4. The results we find are smaller than the available experimental values (the range of values = $160 \text{ ergs/cm}^2 \sim 300 \text{ ergs/cm}^2$). Two possible sources of the discrepancy are the following: our neglect of s-d hybridization and the fact that the measured values refer to nickel in its ferromagnetic state rather than the paramagnetic state which we used in our calculation.

5. Although our value for the stacking fault energy is rather smaller than the best experimental value, it is in much closer agreement than is the value calculated by Cyrot-Lackmann using the moment scheme. Our result is a factor of three higher than her result.

Therefore, the next step in such calculations would be to include s-d hybridization effect for a ferromagnetic state nickel.

Let us finally notice that our scheme could in a straightforward way be used to calculate energies of more complicated defects, for instance, formation energy of vacancies, etc.

Appendix A

In this appendix we present expressions for the integrals used in the computation of the matrix elements of the Hamiltonian.

In the Cartesian coordinates a Gaussian type orbital (GTO) centered at \underline{A} is written as

$$\chi(\underline{A}, \alpha, l, m, n) = \alpha_A^l \alpha_A^m \alpha_A^n \exp(-\alpha r_A^2) \quad (\text{A. 1})$$

Here α_A , β_A and γ_A are the components of a position vector \underline{r}_A relative to \underline{A} , $\underline{r}_A \equiv \underline{r} - \underline{A}$, and l , m and n are "quantum numbers" and are zeroes or positive integers.

First, let us define some notations:

$$\alpha_A^{l_1} \alpha_B^{l_2} = (\alpha_P + \overline{PA}_x)^{l_1} (\alpha_P + \overline{PB}_x)^{l_2} \equiv \sum_j f_j(l_1, l_2, \overline{PA}_x, \overline{PB}_x) \alpha_P^j \quad (\text{A. 2})$$

where \overline{PA}_x and \overline{PB}_x are the x component of the vectors \underline{PA} ($\underline{PA} \equiv \underline{P} - \underline{A}$) and \underline{PB} ($\underline{PB} \equiv \underline{P} - \underline{B}$), respectively.

$$F_2(t) \equiv \int_0^1 u^{2l} \exp(-tu^2) du \quad (\text{A. 3})$$

Then we have the following expressions:

$$S(l_2, m_2, n_2) \equiv \int \chi(A, \alpha_1, l_1, m_1, n_1) \chi(B, \alpha_2, l_2, m_2, n_2) dx dy dz$$

$$= \left(\frac{\pi}{\delta}\right)^{3/2} e^{-\frac{\alpha_1 \alpha_2}{\delta} \overline{AB}^2} \sum_{i=0}^{[(l_1+l_2)/2]} f_{2i}(l_1, l_2, \overline{PA}_x, \overline{PB}_x) \frac{(2i-1)!!}{(2\delta)^i}$$

$$\times \sum_{j=0}^{[(m_1+m_2)/2]} f_{2j}(m_1, m_2, \overline{PA}_y, \overline{PB}_y) \frac{(2j-1)!!}{(2\delta)^j}$$

$$\times \sum_{k=0}^{[(n_1+n_2)/2]} f_{2k}(n_1, n_2, \overline{PA}_z, \overline{PB}_z) \frac{(2k-1)!!}{(2\delta)^k}$$

(A. 4)

where

$$\delta \equiv \alpha_1 + \alpha_2$$

$$\underline{P} = (\alpha_1 \underline{A} + \alpha_2 \underline{B}) / \delta$$

$$(2i-1)!! = 1 \cdot 3 \cdot 5 \cdot \dots \cdot (2i-1) \quad (A. 5)$$

and where $[\chi]$ means "largest integer less than or equal to χ ."

$$\begin{aligned}
& \int \chi(A, \alpha_1, l_1, m_1, n_1) \left[-\frac{1}{2} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) \right] \chi(B, \alpha_2, l_2, m_2, n_2) d\tau \\
&= \alpha_2 \{ 2(l_2 + m_2 + n_2) + 3 \} S(l_2, m_2, n_2) \\
&- 2\alpha_2^2 \{ S(l_2 + 2, m_2, n_2) + S(l_2, m_2 + 2, n_2) + S(l_2, m_2, n_2 + 2) \} \\
&- \frac{1}{2} \{ l_2(l_2 - 1) S(l_2 - 2, m_2, n_2) + m_2(m_2 - 1) S(l_2, m_2 - 2, n_2) \\
&+ n_2(n_2 - 1) S(l_2, m_2, n_2 - 2) \} \quad , \quad (A. 6)
\end{aligned}$$

$$\begin{aligned}
& \int \chi(A, \alpha_1, l_1, m_1, n_1) \frac{1}{|\mathbf{r}_c|} \chi(B, \alpha_2, l_2, m_2, n_2) dx dy dz \\
&= \frac{2\pi}{f} e^{-\frac{\alpha_1 \alpha_2}{f} \overline{AB}^2} \sum_{i,r,u} A_{i,r,u}(l_1, l_2, A_x, B_x, C_x, f)
\end{aligned}$$

$$\times \sum_{j,s,v} A_{j,s,v}(m_1, m_2, A_y, B_y, C_y, f)$$

$$\times \sum_{k,t,w} A_{k,t,w}(n_1, n_2, A_z, B_z, C_z, f) F_w \left(\frac{\overline{CP}^2}{4\epsilon} \right) \quad (A. 7)$$

where $\nu = i + j + k - 2(r + s + t) - (u + v + w)$,

$$\epsilon = \frac{1}{4f}$$

and where

$$A_{i,r,u}(l_1, l_2, A_x, B_x, C_x, f) = (-1)^i f_i(l_1, l_2, \bar{P}_x, \bar{B}_x) \frac{(-1)^u i! P_x^{i-2r-2u} (1/4f)^{r+u}}{r! u! (i-2r-2u)!} \quad (A.8)$$

In Eq. (A.7) the summations with respect to indices i , j and k extend from 0 to $l_1 + l_2$, $[i/2]$ and $[(i-2r)/2]$, respectively. The range of (j, s, v) or (k, t, w) can be easily found in the same way.

$$\int dr_1 dr_2 \alpha_{A_1}^{l_1} \gamma_{A_1}^{m_1} \delta_{A_1}^{m_1} e^{-\alpha_1 r_1^2} \alpha_{B_1}^{l_2} \gamma_{B_1}^{m_2} \delta_{B_1}^{m_2} \frac{1}{|r_2 - r_1|} \\ \times \alpha_{C_2}^{l_3} \gamma_{C_2}^{m_3} \delta_{C_2}^{m_3} e^{-\alpha_3 r_2^2} \alpha_{D_2}^{l_4} \gamma_{D_2}^{m_4} \delta_{D_2}^{m_4} e^{-\alpha_4 r_2^2} \\ = \frac{2\pi^2}{f_1 f_2} \left(\frac{\pi}{f_1 + f_2} \right)^{1/2} \exp\left(-\frac{\alpha_1 \alpha_2}{f_1} \bar{A}\bar{B}^2 - \frac{\alpha_3 \alpha_4}{f_2} \bar{C}\bar{D}^2\right)$$

$$\times \sum_{i_1, i_2, r_1, r_2, u} B_{i_1, i_2, r_1, r_2, u}(l_1, l_2, A_x, B_x, P_x, f_1 | l_3, l_4, C_x, D_x, Q_x, f_2)$$

$$\times \sum_{j_1, j_2, A_1, A_2, v} B_{j_1, j_2, A_1, A_2, v} (m_1, m_2, A_y, B_y, P_y, \delta_1 | m_3, m_4, C_y, D_y, Q_y, \delta_2)$$

$$\times \sum_{k_1, k_2, t_1, t_2, \omega} B_{k_1, k_2, t_1, t_2, \omega} (m_1, m_2, A_3, B_3, P_3, \delta_1 | m_3, m_4, C_3, D_3, Q_3, \delta_2) F_{\omega} \left(\frac{PQ^2}{4\delta} \right)$$

(A. 9)

where $\Delta = i_1 + i_2 + j_1 + j_2 + k_1 + k_2 - 2(r_1 + r_2 + A_1 + A_2 + t_1 + t_2) - u - v - \omega$

$$\delta_1 = \alpha_1 + \alpha_2$$

$$\delta_2 = \alpha_3 + \alpha_4$$

$$P = \frac{\alpha_1 A + \alpha_2 B}{\delta_1}$$

$$Q = \frac{\alpha_3 C + \alpha_4 D}{\delta_2}$$

$$\delta = \frac{1}{4\delta_1} + \frac{1}{4\delta_2}$$

(A. 10)

and where

$$B_{i_1, i_2, r_1, r_2, u} (l_1, l_2, A_x, B_x, P_x, \delta_1 | l_3, l_4, C_x, D_x, Q_x, \delta_2)$$

$$= (-1)^{i_2} f_{i_1} (l_1, l_2, \overline{PA}_x, \overline{PB}_x) f_{i_2} (l_3, l_4, \overline{QC}_x, \overline{QD}_x)$$

$$\times \frac{i_1! i_2!}{(4\delta_1)^{i_1} (4\delta_2)^{i_2} \delta^{i_1 + i_2}} \cdot \frac{(4\delta_1)^{r_1} (4\delta_2)^{r_2} \delta^{2(r_1 + r_2)}}{r_1! r_2! (i_1 - 2r_1)! (i_2 - 2r_2)!}$$

$$\times \{i_1 + i_2 - 2(r_1 + r_2)\}! \frac{(-1)^u \overline{QP}_x^{i_1 + i_2 - 2(r_1 + r_2) - 2u} \delta^u}{u! \{i_1 + i_2 - 2(r_1 + r_2) - 2u\}!}$$

(A. 11)

In Eq. (A.9) the summations with respect to the indices $i_1, i_2, \gamma_1, \gamma_2$, and u extend from 0 to $l_1+l_2, l_3+l_4, [i_1/2], [i_2/2]$ and $[(i_1+i_2)/2 - \gamma_1 - \gamma_2]$, respectively. The range of $(j_1, j_2, \lambda_1, \lambda_2, \nu)$ or $(k_1, k_2, t_1, t_2, \omega)$ can be found in the same way.

Appendix B

The stacking fault energy of a nickel crystal is the difference between the ground state energy of a system with a stacking fault and that of a perfect system:

$$\begin{aligned}
 \Delta E &= E^{\text{SF}} - E^{\text{B}} \\
 &= \epsilon^{\text{SF}} - \epsilon^{\text{B}} \\
 &\quad - \frac{1}{2} \int \frac{n^{\text{SF}}(r) n^{\text{SF}}(r')}{|r-r'|} dr dr' + \frac{1}{2} \int \frac{n^{\text{B}}(r) n^{\text{B}}(r')}{|r-r'|} dr dr' \\
 &\quad + \int n^{\text{SF}}(r) [\epsilon_{\text{xc}}(n^{\text{SF}}(r)) - \mu_{\text{xc}}(n^{\text{SF}}(r))] dr \\
 &\quad - \int n^{\text{B}}(r) [\epsilon_{\text{xc}}(n^{\text{B}}(r)) - \mu_{\text{xc}}(n^{\text{B}}(r))] dr \\
 &= \Delta E_1 + \Delta E_2 + \Delta E_3
 \end{aligned}
 \tag{B.1}$$

where

$$\begin{aligned}
 \Delta E_1 &\equiv \epsilon^{\text{SF}} - \epsilon^{\text{B}} \\
 \Delta E_2 &\equiv -\frac{1}{2} \int \frac{n^{\text{SF}}(r) n^{\text{SF}}(r')}{|r-r'|} dr dr' + \frac{1}{2} \int \frac{n^{\text{B}}(r) n^{\text{B}}(r')}{|r-r'|} dr dr' \\
 \Delta E_3 &\equiv \int n^{\text{SF}}(r) [\epsilon_{\text{xc}}(n^{\text{SF}}(r)) - \mu_{\text{xc}}(n^{\text{SF}}(r))] dr - \int n^{\text{B}}(r) [\epsilon_{\text{xc}}(n^{\text{B}}(r)) - \mu_{\text{xc}}(n^{\text{B}}(r))] \\
 &\quad dr
 \end{aligned}
 \tag{B.2}$$

Here the subscripts SF and B denote the system with the stacking fault and the perfect system respectively.

For a nickel crystal in the $3d^{10}4s^0$ configuration the single particle energy ϵ is given by Eq. (3.6). Then ΔE_1 is given by

$$\Delta E_1 = 1.98 \text{ ergo/cm}^2$$

Since ΔE_2 involves two six-dimensional integrals, usually it is impossible to do this integration numerically. However, in our representation the charge density $\rho(\mathbf{r})$ is expressed in terms of a number of GTO (see Eq. (3.5)) and this integral can therefore be calculated analytically. Due to the large computation time (because the number of GTO is too large) we cannot in practice calculate ΔE_2 directly. Here we want to give some estimates for this term under the assumption that the GWF do not overlap between the third nearest neighbors. If we write $\beta \equiv (\alpha, \mathbf{l}, n)$, the atomic wave functions $\Psi_n^\alpha(\mathbf{r}-\mathbf{l})$ can be written as

$$\Psi_\beta(\mathbf{r}) = \Psi_n^\alpha(\mathbf{r}-\mathbf{l}) \quad (\text{B. 3})$$

The GWF and the electron charge density are given by

$$a_\beta(\mathbf{r}) = \Psi_\beta(\mathbf{r}) - \frac{1}{2} \sum_{\beta \neq \beta'} \Psi_{\beta'}(\mathbf{r}) (\Psi_{\beta'} | \Psi_\beta) \quad , \quad (\text{B. 4})$$

$$\begin{aligned}
 n(r) &= \sum_{\beta} |a_{\beta}(r)|^2 \\
 &= \sum_{\beta} \Psi_{\beta}(r) \Psi_{\beta}(r) - \sum_{\substack{\beta, \beta' \\ \beta \neq \beta'}} \Psi_{\beta}(r) \Psi_{\beta'}(r) (\Psi_{\beta'}, \Psi_{\beta})
 \end{aligned}
 \tag{B.5}$$

Therefore, the coulomb interaction energy can be written as

$$\begin{aligned}
 \int \frac{n(r)n(r')}{|r-r'|} dr dr' &= \sum_{\beta} \sum_{\delta} \int \frac{\Psi_{\beta}(r) \Psi_{\beta}(r) \Psi_{\delta}(r') \Psi_{\delta}(r')}{|r-r'|} dr dr' \\
 &\quad - 2 \sum_{\beta} \sum_{\delta} \sum_{\substack{\delta' \\ \delta \neq \delta'}} (\Psi_{\delta'}, \Psi_{\delta}) \int \frac{\Psi_{\beta}(r) \Psi_{\delta}(r) \Psi_{\delta'}(r') \Psi_{\delta'}(r')}{|r-r'|} dr dr'
 \end{aligned}
 \tag{B.6}$$

The first term on the right hand side of Eq. (B.6) is a two-center integral (β, δ) and the second term is a three-center integral (β, δ, δ'). Since the stacking fault preserves the same number of nearest and second nearest neighbors at the same distance as that in perfect lattice, the two-center integrals give the same values for the system with and without a stacking fault (see Eq. (A.9)). By the same reason, the three-center integrals give the same results for these two different systems except in the following situation: the three centers involve three parallel planes in which the stacking fault occurs. The difference of this kind of term between the system with a stacking fault and the system without a stacking fault is bounded by 0.16 ergs/cm^2 . Therefore, we can neglect the effect of ΔE_2 on the stacking fault energy.

We calculate ΔE_3 using an IMSL three-dimensional integration subroutine, and the result is given by

$$\Delta E_3 = 0.014 \text{ ergo/cm}^2$$

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Figure 1. Flow chart for the calculation of Ni stacking fault energy.

Starting from atomic wave function and densities, we first obtain (a) generalized Wannier function $a_{\underline{g}}^{\alpha}(\underline{r})$ and (b) an effective potential for the stacking fault. From these the Hamiltonian matrix and finally single particle energy, electron density and total energy are calculated.

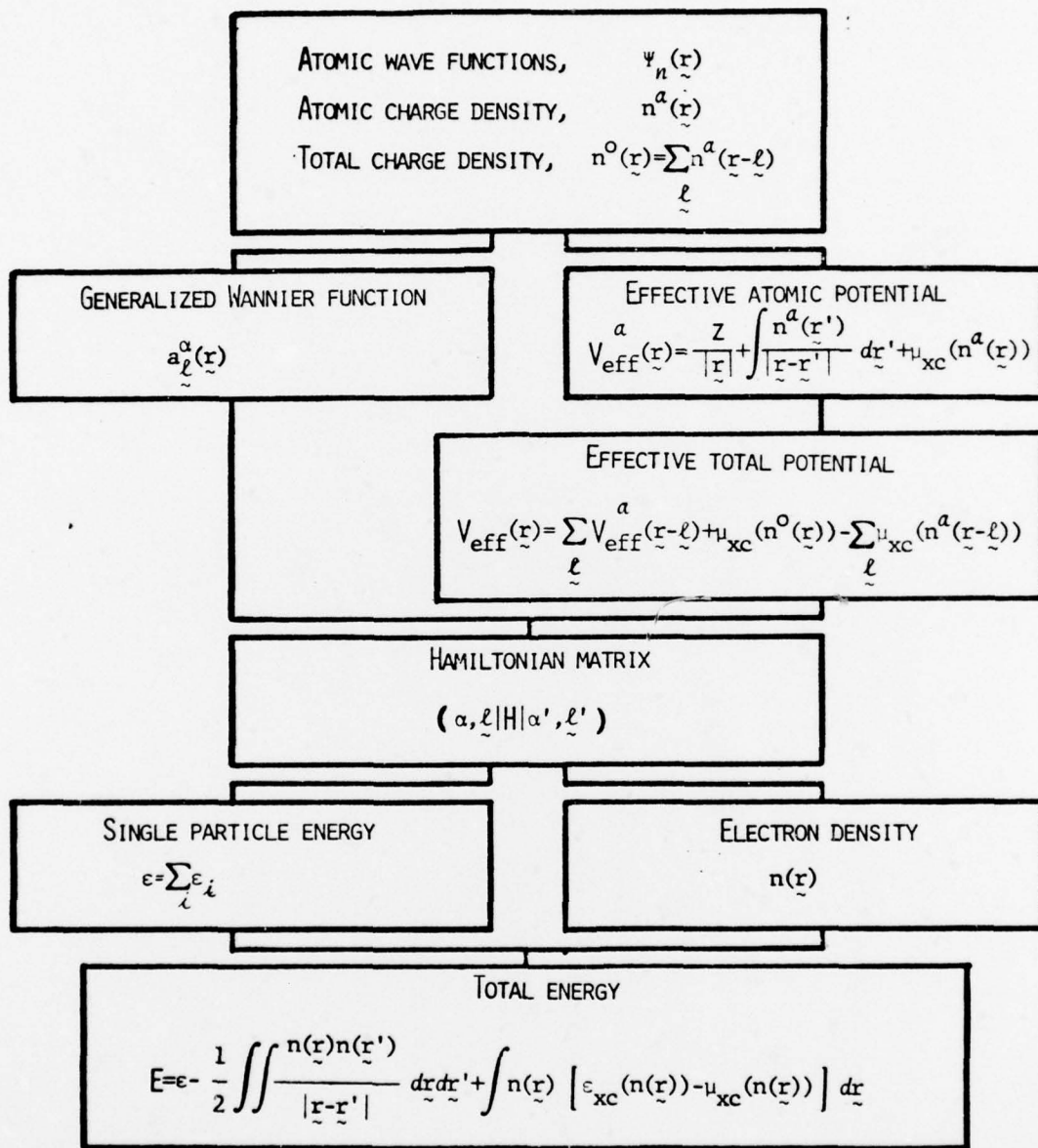


Figure 2(a). Projection normal to the $(1, 1, 1)$ plane showing the three types of stacking positions A, B, and C; (b) Perfect f. c. c. stacking; (c) Intrinsic stacking fault in f. c. c. structure; (d) Extrinsic stacking fault in f. c. c. structure.

Figure 3 (a). The bulk density of states of Ni. The histogram is deduced from Pettifors exact calculations, the full line being our result correct to the 10th continued fraction coefficients.

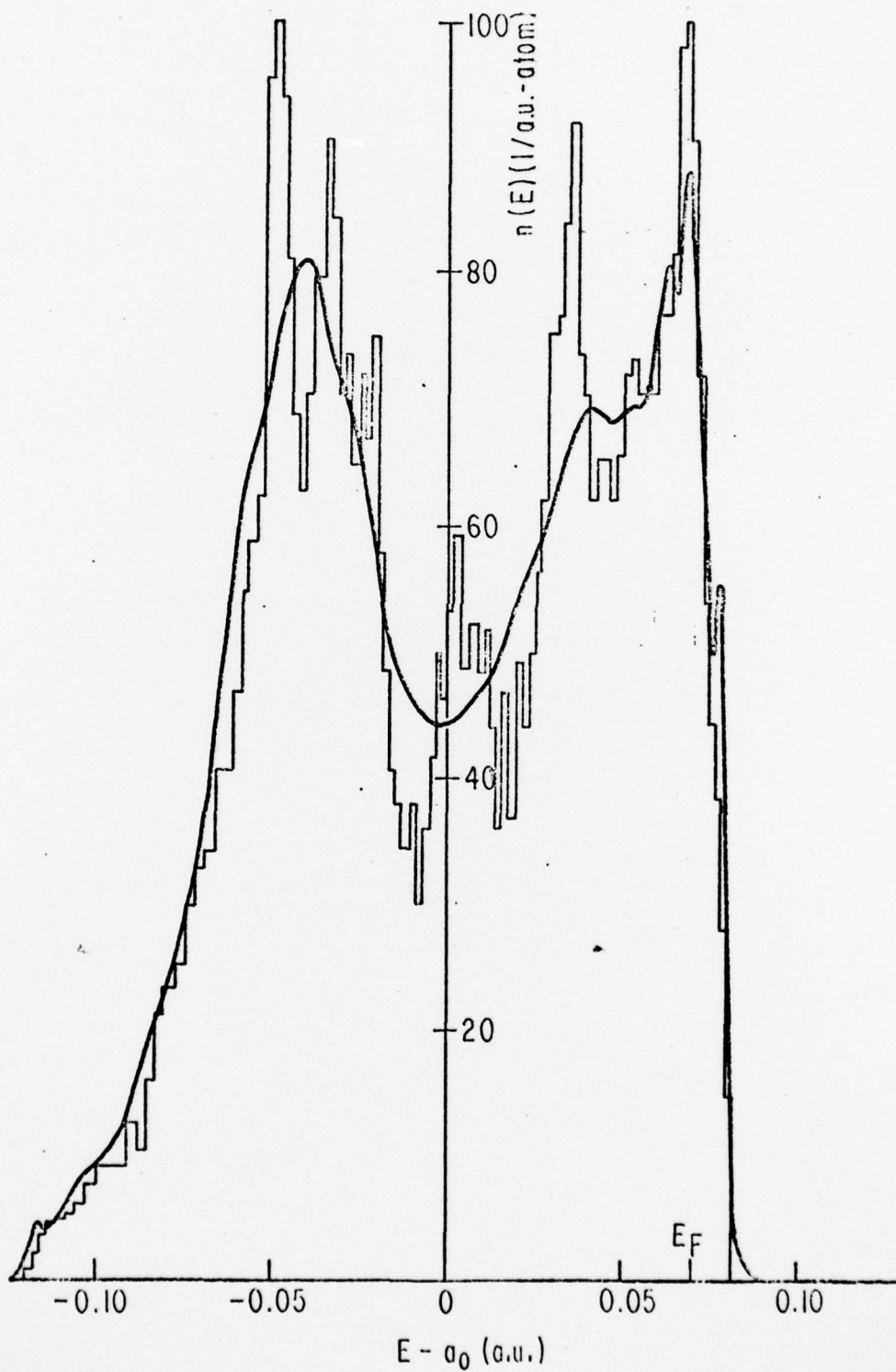


Figure 3 (b). The local density of states on the stacking fault
with $u_0=0$.

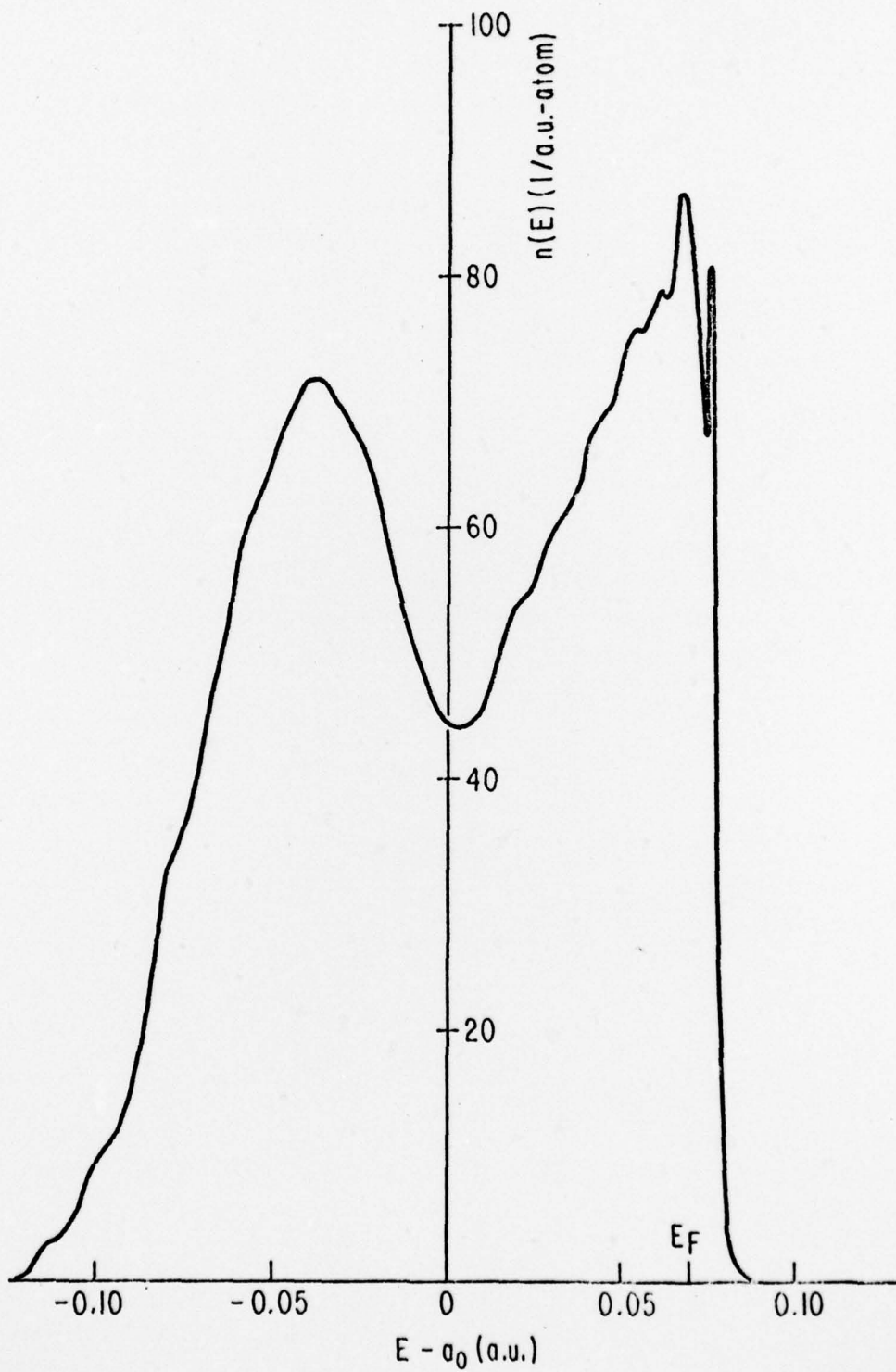


Figure 3(c). The local density of states on the stacking fault with

$$u_0 = 9.80291 \times 10^{-5} \text{ a.u.}$$

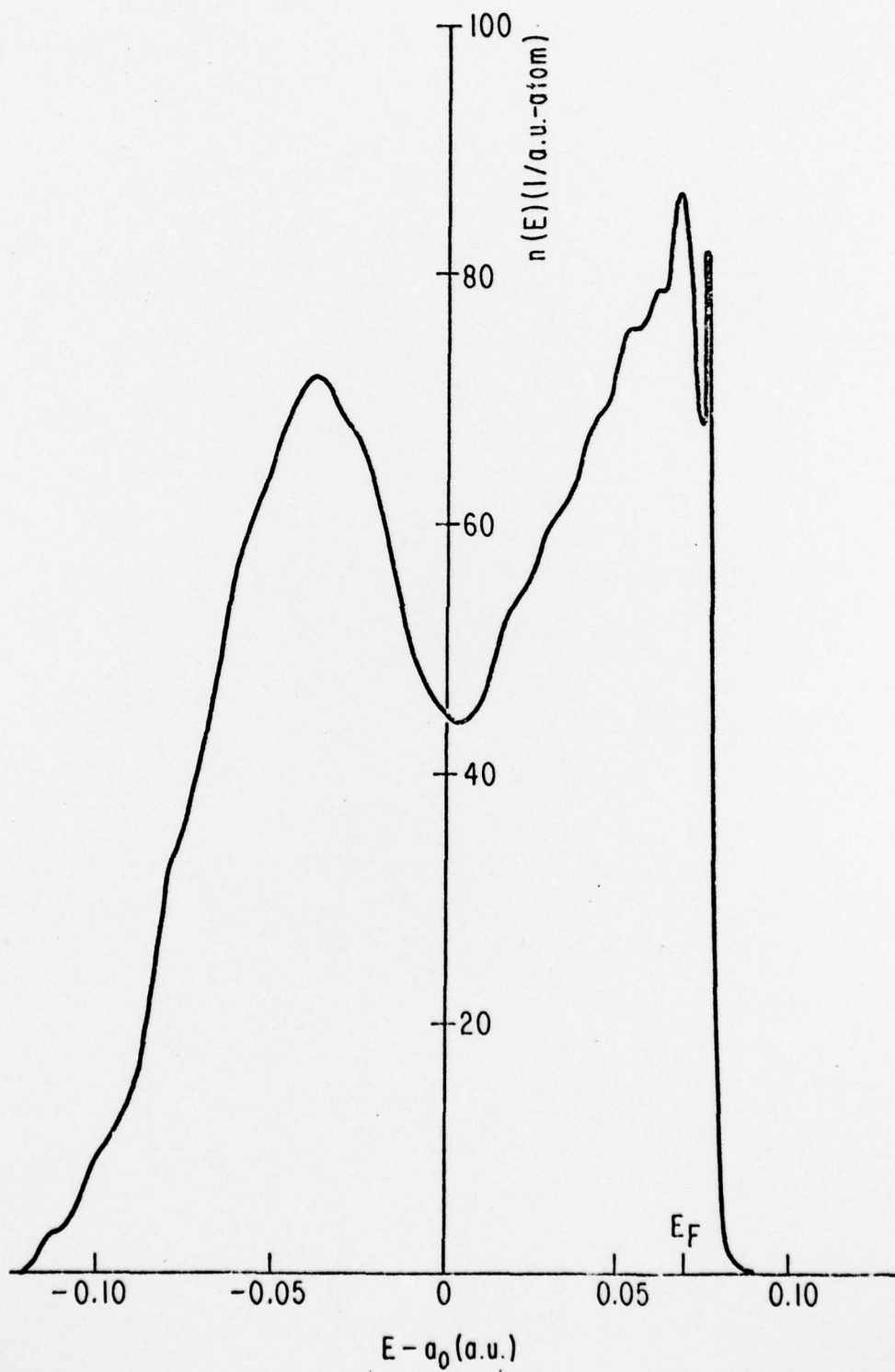


Figure 4. The bulk density of states given by the Edgeworth series
fitted with 4 moments for Ni.

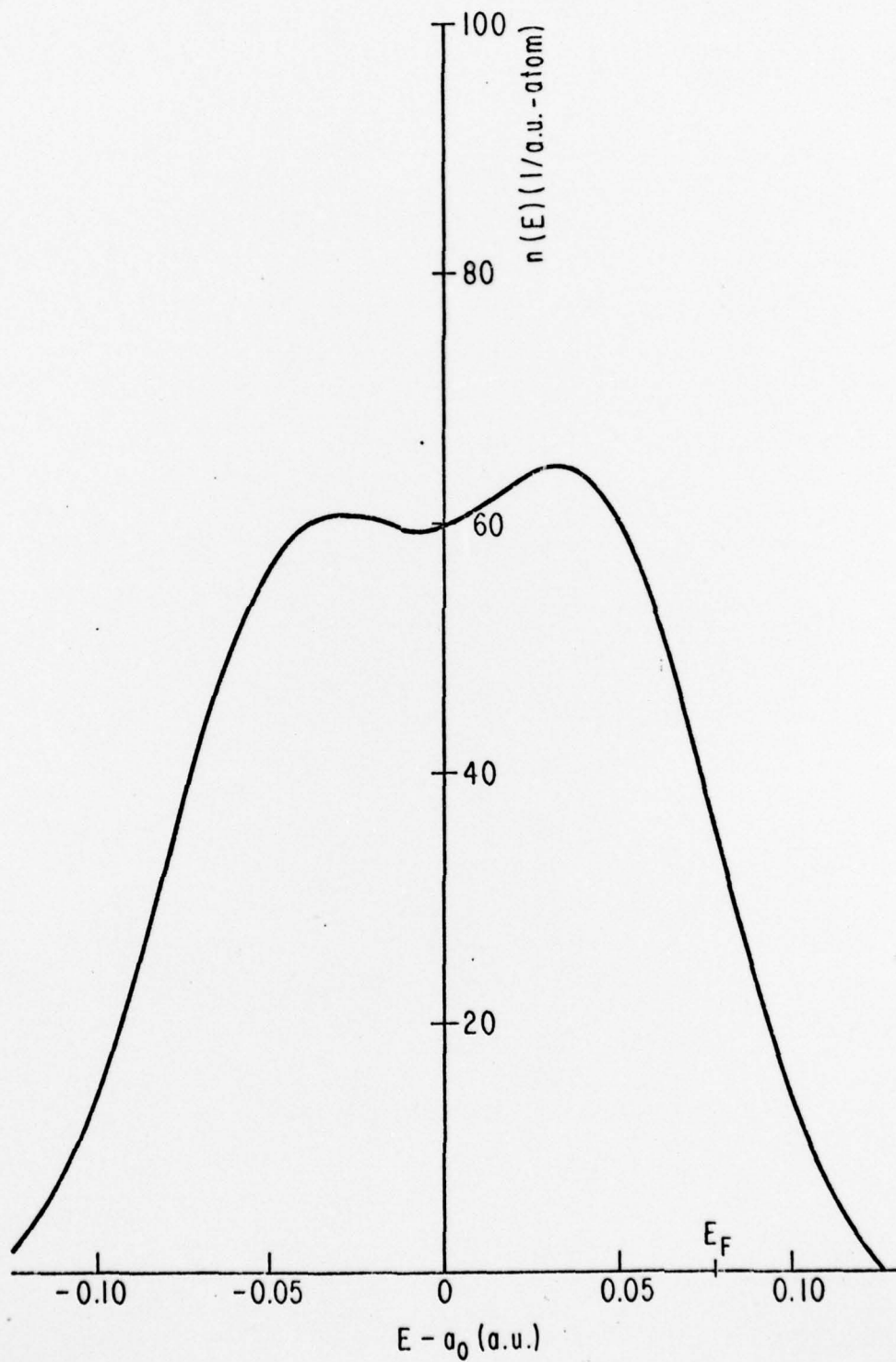


Table 1. Orbital exponential parameters α_i and expansion coefficients C_i for 1s, 2s, 3s, 2p, 3p and 3d orbitals in atomic unit

α_i		C_i	
s	1s	2s	3s
11516.5	33.0481	8.82768	4.20507
3061.22	53.2612	19.3895	5.94182
962.010	40.2191	6.74675	6.48046
530.057	64.2795	32.1637	7.55527
165.397	80.7803	4.20110	19.2241
134.438	-19.0622	28.9506	-6.32380
59.5449	14.3051	-.969386	3.35939
15.1521	-.259403	-14.7299	-12.5191
6.24163	.165880	-3.28423	-.048757
1.39054	-.033213	-.028432	3.56488
p		2p	3p
340.262		116.178	46.2843
155.768		154.761	59.3034
50.4147		127.228	55.0839
20.7513		62.4323	26.2800
7.06297		9.45597	-.526122
2.92262		-.394319	-7.10654
.951675		.035764	-1.23424
d			3d
48.9403			62.747
13.7169			36.546
4.63951			13.677
1.57433			2.6311
.486409			.24164

Table 2. Parameters of atomic effective potential expansion in atomic unit. α_i are the exponential parameters; C_i are the coefficients

α_i	C_i
1.710018091851	-26.39857137242
26.72930960088	17.08366865139
7.640172520328	21.12143227226
2.324012025830	32.21210656087
0.260972626075	-0.861105554065

Table 3. Comparison between the stacking fault energies in ergs/cm² which are obtained by the moments scheme, the non-self-consistent scheme and the self-consistent scheme by using (a) our constructed non-periodic Hamiltonian, (b) 3 parameters $dd\sigma$, $dd\pi$ and $dd\delta$ fitted Hamiltonians.

	Moments	N. S. C.	S. C.
a	18.50	60.20	64.27
b	20.72	56.40	64.83