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"First principles tight binding approach for alloy electronic structure calculations"

PART I

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Part 1

FIRST PRINCIPLES TIGHT BINDING APPROACH FOR ALLOY ELECTRONIC STRUCTURE CALCULATIONS

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Introduction

Electronic structure calculations of (a) ordered alloys in $\underline{k}$-space (supercell) or (b) disordered alloys (either topological or substitutional) in real space, necessitate localized basis functions which are more atomic-like than free-electron like. Tight-binding (TB) or LCAO-type methods are known to be most suitable for the study of cohesion and phase stability of alloys, especially when the overlaps of the atomic wave functions are <u>not</u> too large. Different TB approaches may be broadly categorized as (a) phenomenological i.e. parameters obtained from fits to electron bands /1/ and (b) first principles viz. the TB-LMTO method proposed by Andersen and Jepsen /2/. The former is simple and easily amenable to complicated structures, for example, the empirical Slater-Koster(SK) parameters are very useful to throw light on the underlying physical mechanism. The latter yields more accurate results for density of states, charge density, total energy etc. Also the SK parameters, obtainable from TB-LMTO without any empirical fitting, are valid

over a wide range of interatomic separation through explicit charge self-consistency, and are 'transferable' with changes in structural and chemical environments /3/. By properly accounting for the dependence of SK parameters on the interatomic distance (d), one can 'scale' the band structure for different lattice spacings without performing fresh calculations every time. The distance dependence of the empirical TB matrix elements is given by /4/

$$V_{ll'm} = C_{ll'm} \left(\frac{d}{\omega}\right)^{-\eta}$$

where $C_{ll'm}$ is a constant (volume independent for a particular element and ω is a scaling constant (may be chosen as the Wigner-Seitz radius) for making 'd' dimensionless; the exponent η had been empirically fitted /4 as $\eta = 2$ for s-s, s-p and p-p, $\eta = 7/2$ for s-d and p-d, $\eta = 5$ for d-d.

Andersen, on the other hand, arrived at a similar scaling law, based on LMTO /5/ viz.

$$V_{ll'm} = C_{ll'm} \left(\frac{d}{\omega}\right)^{-(l+l'+1)}$$

and subsequently introduced a 'screening transformation' /2/ to make it fall exponentially

The TB-LMTO hamiltonian, in its simplest form, consist of just two terms viz. an on-site term ϵ_i^{λ} and a 2-centre hopping term $\beta_{ij}^{\lambda\mu}$, making it extremely attractive to be deployed by alloy theorists during the last 10 years. In this talk I shall summarize only the salient features of this method, whose details may be obtained from the original papers and review articles written by Andersen and his coworkers /see refs. 6 and 7 for ex./. The latest LMTO version in the TB representation has been discussed in details in ref. 8, which also includes many of the recent developments in this field. As far as applications to alloys are concerned TB-LMTO has been successfully hooked up with (a) CPA by Kudrnovsky /9/, Singh & Goms, Razee and Prasad /10/ and others (b) recursion method by Vergas /12/, Bose /13/ and others and (c) Augment space Recursion by Mookerjee and coworkers /14/. All these applications so far are based on the simplifying atomic sphere approximation (ASA), although it is now desirable that a 'screened' (or TB version of full potention LMTO be used to arrive at the precise energetics of alloys.

2. First principles tight binding LMTO method

For a quick 'warm-up' on the LMTO formalism, we start with the so-called "envelope function", which is a spherical wave (Hankel function) in case of LMTO and its descendent ASW method, and a plane wave in case of LAPW method. The envelope function is defined as the solution of the wave equation in the interstitial region with constant potential V_0

$$\left(\nabla^2 + K^2\right) \chi^i(K, \underline{r}) = 0 \qquad (1)$$

where $K^2 = E - V_0$ is the kinetic energy of the interstitial region. It has two solution viz. the regular solution $J^0_{RL}(K, \underline{r})$, ~~Bessel fn~~ and the irregular solution $N^0_{RL}(K, \underline{r})$, which are nothing but the Bessel and Neumann functions (multiplied by spherical harmonics). If K^2 is negative, n_l diverg. as $e^{|K|r}/r$ and in that case one can define ~~as~~ a decaying Hankel function K^0_l which is a linear combination of j_l and n_l. K^0's can be expanded in terms of J^0's a

$$K^0_{RL}(K, r) = -\sum_{L'} J^0_{R'L'}(K, r)\, S^0_{R'L', RL} \qquad (2$$

where S^0's are the bare canonical structure constants.

"Canonical" means S^0 is independent of energy, potential and scale; "Bare" implies unscreened i.e. extended in space.

Andersen first postulated /15/ that one can disregard the energy variation of κ^2 and use instead a single characteristic K^2-value (energy independent) so that there is restricted variational freedom in the interstitial region. This approximation is valid provided the 'wavelength' $2\pi/K$ is large in the interstitial.* A further drastic simplification takes place by setting $K^2 = 0$ and letting the muffin-tin spheres inflate to space filling (and hence slightly overlapping) atomic spheres. This is ASA, under which the wave eq^n (1) boils down to Laplace's eq^n

$$\nabla^2 \chi^i_{RL}(\underline{r}_R) = 0 \qquad \text{——— (3)}$$

whose solution

$$\chi^i_{RL}(\underline{r}_R) = \left(a_1 r_R^{\ell} + a_2 r_R^{-\ell-1}\right) Y_L(\hat{r}_R) - ($$

has a long-ranged tail $K^0_{RL} \sim r_R^{-\ell-1}$
Summation of such long-ranged tail is rather difficult in real space.

So there have been attempt to "localize" the "tails" by appropriate screening of the envelope functions. This so-called TB basis set can be constructed from short-ranged linear combination of conventional basis set /2,6/. Introducing some "screening numbers" α_l which is a diagonal matrix (usually independent of R), one can define the screened quantities K^α, J^α and S^α ~~cor~~ analogous to the corresponding unscreened ($\alpha = 0$) quantities in eqn (2) i.e.

$$K^\alpha_{RL}(K, r_R) = -\sum J^\alpha_{R'L'}(K, r_{R'}) S^\alpha_{R'L', RL} \quad -(5$$

where $|J^\alpha\rangle = |J^0\rangle - \alpha |K^0\rangle$ —— (6

Using the superscript "∞" to imply a function extended in all space, the "unscreened" multi-pole field can be written as

$$|K^0\rangle^\infty = |K^0\rangle - |J^0\rangle S^0 \quad — (7)$$

Corresponding screened multi-pole field

$$|K^\alpha\rangle^\infty = |K^0\rangle - |J^\alpha\rangle S^\alpha$$

$$= |K^0\rangle (1 + \alpha S^\alpha) - |J^0\rangle S^\alpha \quad -(8)$$

In order for (8) to be superposition of (7)

i.e. $|K^\alpha\rangle^\infty = |K^0\rangle^\infty (1 + \alpha S^\alpha)$ — (9)

the screened structure matrix S^α should satisfy the Dyson's eqn

$$S^\alpha = S^0(1 + \alpha S^\alpha) \quad \text{——} \quad (10a)$$

Here αS^α can be designated as the "screening charge" /16/

One can also rewrite (10) in the form

$$S^\alpha = (1 - \alpha S^0)^{-1} \quad \text{——} \quad (10b)$$

where one has to do explicit inversion of the matrix $(1-\alpha S^0)$, instead of solving the Dyson's eqn (10a) iteratively. S^α can be evaluated both in real space and in k-space, and has an exponentially decaying form

$$S^\alpha = A \exp\left(-\lambda^\alpha \frac{d}{w}\right) \quad \text{——} \quad (11)$$

and is found to be "universal" for some optimum choice of the screening numbers α_l. For spd screening, for example, these numbers were found by trial and error /2/ to be

$\alpha_0 = 0.3485$, $\alpha_1 = 0.05303$, $\alpha_2 = 0.01071$, $\alpha_l = 0 \; \forall l \geq 3$

Augmentation and MTO basis

The envelope functions discussed above can serve as basis orbitals only in the regions away from the atomic cores, where the potential is sufficiently flat. As we come closer to the nucleus, the ~~potential~~ electrostatic potential of the atomic core is almost spherically symmetric. This region can be described by the so-called "augmentation spheres" within which the Kohn-Sham equation with spherical potential $V_R^{eff}(r)$ is

$$\left[-\nabla^2 + V_R^{eff} - E\right] \phi_{Rl}(E, r_R) = 0 \qquad -(12$$

The partial wave solutions ϕ_{Rl} are orthonormalized within the atomic spheres and we emphasize this by introducing the orthogonal (γ) representation ϕ^{γ}_{Rl}

$$\left.\begin{aligned} \langle \phi^{\gamma} | \phi^{\gamma} \rangle &= \int_0^{s_R} [\phi^{\gamma}_{Rl}(E,r)]^2 r^2 dr = 1 \\ \langle \phi^{\gamma} | \dot{\phi}^{\gamma} \rangle &= \int_0^{s_R} \phi^{\gamma}_{Rl}(E,r)\, \dot{\phi}^{\gamma}_{Rl}(E,r)\, r^2 dr = 0 \end{aligned}\right\} (1$$

Again these partial waves are long-ranged ($\sim r^l$) and hence not very convenient as basis.

Therefore the so-called muffin-tin orbitals (MTO) were introduced [15], which are nothing but linear combinations of ϕ and $\dot{\phi}$.

In generalized (α-) representation

$$\chi^{\alpha}_{RL}(E, r_R) = \phi^{\alpha}_{RL}(E, r_R) + \sum_{R'L'} \dot{\phi}^{\alpha}_{R'L'}(E, r_{R'})\, h^{\alpha}_{R'L', RL}(E) + K^{\alpha}_{RL}(E, r_R) \qquad -(14)$$

where

$$\phi^{\alpha}_{Rl}(E, r_R) = \phi^{\gamma}_{Rl}(E, r_R) \frac{N^{\alpha}_{Rl}(E)}{N^{\alpha}_{Rl}} \qquad -(15)$$

$$\dot{\phi}^{\alpha}_{Rl}(E, r_R) = \dot{\phi}^{\gamma}_{Rl}(E, r_R) \frac{N^{\alpha}_{Rl}(E)}{N^{\alpha}_{Rl}} + \phi^{\gamma}_{Rl}(E, r_R) \frac{\dot{N}^{\alpha}_{Rl}(E)}{N^{\alpha}_{Rl}} \qquad -(16)$$

$K^{\alpha}_{RL}(E, r_R)$ is the interstitial Hankel function envelope (truncated inside all MT spheres)

$$h^{\alpha}_{R'L', RL}(E) = -\left[\dot{P}^{\alpha}_{R'l'}(E)\right]^{-\frac{1}{2}} \left[P^{\alpha}_{R'L'} S_{RR'} \delta_{LL'} - S^{\alpha}_{R'L', RL}\right] \left[\dot{P}^{\alpha}_{Rl}(E)\right] \qquad -(17)$$

where P^{α}, the potential function is a diagonal matrix defined as

$$P^{\alpha}_{l}(E) = P^{0}_{l}(E)\left[1 - \alpha P^{0}_{l}(E)\right]^{-1} \qquad -(18)$$

with $P^{0}_{l}(E) = 2(2l+1)\dfrac{D_l(E) + l + 1}{D_l(E) - l}$

$$D_l(E) = \frac{\partial \ln \phi_l(E, r)}{\partial \ln r}\bigg|_{S_R} = \frac{r \phi_l'(E, r)}{\phi_l(E, r)}\bigg|_{S_R}$$

Linearization of MTO's

The shapes of MTO's depend on energy and also they diverge at the sites. Both these can be 'healed' by introducing energy linearization. If we expand the energy dependence of the radial wave function in a Taylor's series w.r.t. an arbitrary expansion energy E_ν,

$$|\phi(E,r)\rangle = |\phi(E_\nu,r)\rangle + |\dot{\phi}(E_\nu,r)\rangle (E-E_\nu) + |\ddot{\phi}(E_\nu,r)\rangle \frac{(E-E_\nu)^2}{2} + \cdots \quad (19)$$

and truncate after the linear term, we can still describe fairly well the change of the radial wave function throughout the atomic sphere ($r \le s_R$). Thus the linear MTO's or LMTO's are defined as the 'healed' MTO's with $E = E_\nu$ and $\kappa^2 = \kappa_\nu^2$. They match with the exact MTO's i.e. $\chi^\alpha_{RL}(E, r_R) \longrightarrow \chi^\alpha_{RL}(E_\nu, r_R)$ to linear order in $E - E_\nu$.

$$\left.\begin{aligned} &\text{At } E = E_\nu, \quad |\phi^\alpha\rangle = |\phi^\nu\rangle = |\phi\rangle \\ &\text{and} \quad |\dot{\phi}^\alpha\rangle = |\dot{\phi}^\nu\rangle + |\phi\rangle o^\alpha \end{aligned}\right\} \quad (20)$$

where $o^\alpha = \dot{N}^\alpha / N^\alpha = \langle \phi | \dot{\phi}^\alpha \rangle$

& $p^\alpha = (o^\alpha)^2 + p^\nu \; ; \; \langle \dot{\phi}^\alpha | \dot{\phi}^\alpha \rangle \longrightarrow$ "small" parameter

Thus the LMTO basis can be written as

$$|\chi^\alpha\rangle = |\phi\rangle + |\dot{\phi}^\alpha\rangle h^\alpha + |K^\alpha\rangle \quad -(21)$$

where $h^\alpha = -P^\alpha(\dot{P}^\alpha)^{-1} + (\dot{P}^\alpha)^{-\frac{1}{2}} S^\alpha (\dot{P}^\alpha)^{-\frac{1}{2}}$

$$= (C^\alpha - E_\nu) + (\sqrt{\Delta^\alpha}\, S^\alpha \sqrt{\Delta^\alpha}) \quad -(22)$$

E_ν, C^α, Δ^α being known as the "potential parameters" which can be expressed in terms of the potential function P^α as

$$\left.\begin{aligned} C^\alpha - E_\nu &= -P^\alpha/\dot{P}^\alpha \\ \Delta^\alpha &= (\dot{P}^\alpha)^{-1} \\ \alpha &= (P^0)^{-1} - (P^\alpha)^{-1} \end{aligned}\right\} \quad -(23)$$

Here S^α is the only non-diagonal matrix.

Thus the multi-centered MTO's have been constructed from the single centered partial waves ϕ and $\dot{\phi}$ and the corresponding potential parameters. The expression (21) may be regarded as the linear term in the Taylor series and hence the name LMTO.

Invoking ASA further simplifies (21) by dispensing with the interstitial function K^α and ~~one~~ we are left with only two adjustable quantities viz C^α and h^α which can be chosen such that the augmentatio are continuous and differentiable at sphere bounda

Hamiltonian and Overlap matrices within ASA

$$O^\alpha = \langle \chi^\alpha | \chi^\alpha \rangle = (1 + h^\alpha o^\alpha)(1 + o^\alpha h^\alpha) + h^\alpha p^\alpha h^\alpha \quad \text{— (24a}$$

$$H^\alpha = \langle \chi^\alpha | -\nabla^2 + V_R^{eff} | \chi^\alpha \rangle$$

$$= (1 + h^\alpha o^\alpha) h^\alpha + (1 + h^\alpha o^\alpha) E_\nu (1 + o^\alpha h^\alpha) + h^\alpha E_\nu p^\alpha \quad \text{— (24b}$$

Dropping terms $h^\alpha p^\alpha h^\alpha$ and $h^\alpha E_\nu p^\alpha h^\alpha$ which involve the small parameter p^α, and invoking löwdin orthonormalization prescription, we get

$$H = (O^\alpha)^{-\frac{1}{2}} H^\alpha (O^\alpha)^{-\frac{1}{2}}$$

$$= E_\nu + h^\alpha (1 + o^\alpha h^\alpha)^{-1}$$

$$= E_\nu + h^\alpha - h^\alpha o^\alpha h^\alpha + \cdots \quad \text{— (25)}$$

Thus the Löwdin orthonormalized hamiltonian can be expressed as a power series in h^α, which is the effective two-centre TB hamiltonian (22). The corresponding new basis set

$$|\chi^\gamma\rangle = |\chi^\alpha\rangle (1 + o^\alpha h^\alpha)^{-1} \quad \text{— (26}$$

is orthogonal to first order in h^α

[similarly define $h^\gamma = h^\alpha (1 + o^\alpha h^\alpha)^{-1}$]

By dropping terms in (25) which are of higher order in h^α, one gets the simplest form of first order Hamiltonian

$$\mathcal{H}^{(1)} = E_\nu + h^\alpha$$
$$= C^\alpha + \sqrt{\Delta^\alpha}\, S^\alpha \sqrt{\Delta^\alpha} \qquad \text{— (27)}$$

which is most widely used for first principles calculation on alloys, since it is in the Ising form with an on-site or diagonal terms $\epsilon_i^\lambda \equiv C^\alpha$ and a two-centre hopping term $\beta_{ij}^{\lambda\mu} \equiv \sqrt{\Delta^\alpha} S^\alpha \sqrt{\Delta^\alpha}$

If we use $\mathcal{H} = \mathcal{H}^{(1)} - h^\alpha o^\alpha h^\alpha$, the range of Hamiltonian is approximately twice that of $\mathcal{H}^{(1)}$ and the resulting DOS features will have positions correct to $(E - E_\nu)^2$. Therefore one can control the effect of truncating the range of $\mathcal{H}$ in LMTO.

Charge density and ASA total energy

The LMTO-ASA eigenvalue equation for a crystalline solid can be written as

$$\mathcal{H}(k)\, u_j(k) = E_j(k)\, u_j(k) \qquad -(28)$$

where $\mathcal{H}$ is given by (25) or (27) depending on the order of approximation in the Hamiltonian

The basis orbitals (in Fourier space) are the Bloch sums of LMTO's

$$\chi^{\gamma}_{RL}(k) = \sum_{T} e^{ik.T}\, \chi^{\gamma}_{RL}(r-R-T) \qquad -(29)$$

In terms of the eigenvectors $u_j(k)$, we can expand the wave function $\psi_j(k,r)$ of the crystal (correct to first order in $E_j - E_\nu$) as

$$\begin{aligned}\psi_j(k,r) &= |\chi^{\gamma}(k)\rangle\, u_j(k) \\ &= [|\phi\rangle + |\dot{\phi}^{\gamma}\rangle h^{\gamma}(k)]\, u_j(k) \\ &= [|\phi\rangle + |\dot{\phi}^{\gamma}\rangle (E_j(k) - E_\nu)]\, u_j(k)\end{aligned} \qquad -(30)$$

Corresponding energy eigenvalues

$$E_j^{(2)} = u_j^{+}\, \mathcal{H}^{(2)}\, u_j$$

are correct to order $(E_j - E_\nu)^2$

and the density matrix

$$n = \sum_j \int d\underline{k}\; u_j(k)\, f(E_j(k))\, u_j^{\dagger}(k) \qquad -(31$$

where $f(E)$ is the Fermi function.

The spherically averaged valence electron charge density $n_R(r)$, needed to construct the ASA potential is given by

$$n_R(r) = \frac{1}{4\pi} \sum_l \Big[m_{Rl}^{(0)} \phi_{Rl}(r)^2 + 2 m_{Rl}^{(1)} \phi_{Rl}(r) \dot{\phi}_{Rl}($$

$$+ m_{Rl}^{(2)} \{ \dot{\phi}_{Rl}(r)^2 + \phi_{Rl}(r)\, \ddot{\phi}_{Rl}(r) \} \Big]$$

$$-(32)$$

where the q $\underline{\text{th}}$ moment is defined as

$$m_{Rl}^{(q)} = \sum_{j,\underline{k}}^{occ} \left[E_j(k) - E_{\nu,Rl} \right]^q \sum_m |u_{RL,j}(k)|^2$$

$$-(32a)$$

Actually, the core electron contribution has to be added to this valence electron density (32) in order to generate the total spheridized electron density, let us call it $n_R(r)$.

The resulting one electron ASA potential in the sphere at R is

$$V_R^{eff}(r) = \left[2 \int_0^{s_R} \frac{n_R(r)}{|r-r'|} 4\pi r'^2 dr' - \frac{2Z_R}{|r-R|} + \mu_{xc}(n_R(r)) \right] - \sum_{R \neq R'} \sum_T \frac{2Q_R}{|R-R'-T|}$$

$$= V_{sphere} + V_{Madelung} \quad -(33)$$

where $$Q_R = -\int_0^{s_R} 4\pi r^2 n_R(r) dr + Z_R \quad -(33a)$$

The ASA total energy (per unit cell) of the valence electrons and ions is

$$E_{tot} = T_{kin} + \sum_R U_R + \sum_R \sum_{R'}{}' Q_R Q_{R'} \sum_T |R-R'-T|^{-1} \quad -(34)$$

where

$$T_{kin} = \sum_{j,k} f(E_j) E_j(k) - \sum_R \int_0^{s_R} V_R(r) n_R(r) 4\pi r^2 \quad -(34a)$$

& $$U_R = \int_0^{s_R} n_R(r) V_{sphere}(r) 4\pi r^2 dr \quad -(34b)$$

It is to be noted that the total energy expression (34) is ~~inexact as~~ it has within the integrals, the quantity $n_R(\underline{r})$ which is the sphere charge density within ASA and not the true charge density $n(\underline{r})$. In ASA we have neglected (a) the interstitial region (b) the non-spherical parts of the potential $V^{eff}(\underline{r})$ and (c) the higher partial waves. Part of the error involved in sphendization can be salvaged by incorporating the so-called 'combined correction' term /7/ or by generalizing ASA to a non-zero (but fixed) K-value /17/. For close packed metallic solids the error involved in total energy gets cancelled while evaluating differences like compound formation energy etc. But a full potential calculation is essential to find energetics due to symmetry lowering displacements.

3. Full potential LMTO

In spite of all the advantages and simplicity of LMTO-ASA, it suffers from the limitation that it can not yield elastic constants and phonon frequencies which are associated with lattice deformations or symmetry lowering displacements of atoms. Therefore various attempts have been made to develop full potential (FP)-LMTO methods /18-22/ which avoids sphere dization in the self-consistency cycle (i.e. no shape approximation). Weyrich[19] for example, suggested the use of Fourier transform for LMTO's in the interstitial region. This does not increase the size of the hamiltonian and overlap matrices, but makes the construction of charge density tedious. Methfessel /20/ has proposed a technique for handling the full density in all space. Using the values and gradients at the spheres, the product of two LMTO's is fitted by linear combination of two Hankel function and thus the charge density can be found by extrapolation

Savrasov /22/ has recently developed a FP-LMTO method where the integrals over all space are performed as sums of integrals over cells. Each cell integral is performed as a surface integral and thus avoids the slowly converging spherical-harmonics expansion of the cellular step function.

Unfortunately none of these full potential schemes mentioned above use localized orbitals and hence are not quite suitable for alloys (See discussion in reference 8). A direct calculation of charge density via real space TB representation was done by Blöchl /21/. Since localized basis set allows calculation of the matrix elements in real space, this part increases only linearly with the size of the system; the computational effort will be dominated by the diagonalization for systems with more than a few tens of atoms. In Blöchl's approach one can split up the LMTO basis orbitals χ^k into a smooth or pseudo-LMTO part $\tilde{\chi}^k$

which extends over the entire space, and a strongly varying part $\hat{x}^k$ which is localized inside the augmentation spheres. $\hat{x} = x^1 - \tilde{x}^1$, where x^1 & $\tilde{x}^1$ denote the one centre expansions of x and $\tilde{x}$ respectively. $\hat{x}$ is continuous and differentiable everywhere and vanishes at the sphere boundary. Similarly the charge density can be expressed as a sum of a smooth and local parts $n = \tilde{n} + n^1 - \tilde{n}^1$.

The expressions for kinetic energy, electrostatic potential energy and exchange correlation energy become somewhat complicated and may be found in ref. 21. This FP-LMTO method has been successfully used to calculate structural energy differences and phonon frequencies in Si and compared with other approaches /23/. It has also been used to study schottky barrier heights in $NiSi_2$/Si (111) interfaces using supercell geometry /24/. Applications of FP-LMTO for tackling alloy electronic structure is still an open problem.

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