



Augmented Space Recursion Method for the Study of Electronic States of Binary Alloys

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Abstract

We have studied here the electronic structure of pure random disordered alloys formed by Ni with Cu and Au at different ratios by using the linearized tight-binding muffin-tin Orbital (TB-LMTO) method. We also used the recursion technique together with augmented space formalism for increasing the efficiency and the accuracy to calculate the component projected density of states. From the density of state, we can understand the Fermi energy, magnetic moment and binding energy at different alloy compositions. The band structure can be calculated from here also. These studies are helpful for experimentalists and metallurgists in designing materials and alloys with specific properties.

Key words: Electronic structure, Alloys, TB-LMTO, Density of states, Augmented space recursion

Introduction

Among the solid materials, metals are of great interest. For example iron is used in automobiles, copper in electric wiring, where as gold and silver are used in jewelry. These and other metals have played a very important role in the development of our technological world from early historical time to the present and will continue to do so in the future. The explanation of characteristic metallic properties is important to a metallurgist or an engineer who wishes to use metals for practical purposes and to a physicist who is interested in understanding the microscopic structure of materials.

The tight-binding or screened version of the linearized muffin-tin-orbitals method (TB-LMTO) has provided an excellent starting point for first principles electronic structure determination of disordered alloys. The resulting Hamiltonian is short-ranged and therefore ideally provides the extension from the traditional adhoc tight-binding ideas into a fully-self-consistent first principles theory. The basis of the method has been described in detail (Andersen *et al.*, 1994) and relevant details necessary for disordered alloys are given in (Anderson and Japsen *et al.*, 1984). The study of electronic structure of disordered alloys is of great scientific and technological importance. Theoretical approaches have achieved considerable success through the development of mean-field approximations, the most successful of which is

the coherent potential approximation (CPA) (Pinski, *et al.*, 1991). Other techniques include super-cell approaches, attempted generalizations of the CPA and an alternative order-N Green's function technique (Abrikosov *et al.*, 1996). The former is based on the self-consistent determination of a uniform medium to represent the substitutional alloy. The corresponding effective Hamiltonian is lattice transitionally symmetric and its Green function is a good approximation of the configurational averaged Green function. Of the later, the super-cell method is based on the study of different selected ordered structures at various concentrations. In these calculations a large unit cell is constructed which contains different possible configurations and is repeated to generate the entire lattice. The result of such a method contains the artifact of imposed lattice symmetry, which is OK provided we concentrate on the local properties at the centre of the super-cell whose size is rather large. There is no straight-forward rule for constructing a super-cell and in realistic calculations it becomes computationally expensive. A large number of generalizations of the CPA are beset with analytical difficulties and their effective medium is often not translationally symmetric. The only really successful generalization with analytical and translational properties is the traveling cluster approximation of (Kaplan *et al.*, 1981).

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Augmented space theorem and the recursion method [6] carried out in a minimal basis set of the tight-binding linear muffin-tin orbitals method (TB-LMTO) (Andersen et al., 1994; Andersen *et al.*, 1984 and Andersen 1971) in which the Hamiltonian is sparse. The AST states that the configuration average of a well behaved function of a set of random variables is a particular matrix element of the operator obtained by replacing the random variables in the function by the corresponding operators, whose spectral densities are the probability densities of the random variables. The underlying space in which the operator is defined is the space of all possible configurations of the random variables. For example, if the set of random variables have binary distributions, then this configuration space is isomorphic to the configuration space of a set of Ising spin-half objects. The theorem is exact and approximations are introduced only in the calculation of matrix element. The recursion method with a terminator approximation allows us to take into account effects of random environments of a site. The size of this environment depends upon the number of recursion steps we can carry out exactly and the far environment is approximated by the terminator.

Method

The LMTO method for self-consistent calculations of electronic structures of solids was introduced by Andersen and Jepsen (Andersen *et al.*, 1984). It has been described in great detail in a recent monograph (Andersen, 1995]. We shall indicate here only those points which are of specific importance for the present work. We stress here that the transformation of the canonical LMTO into a first principles tight-binding method with a sparse Hamiltonian representation is essential for an effective use of the recursion technique which is the basis of our methodology.

In LMTO representation within atomic sphere approximation, the basis functions have the form

$$\chi_{RL}^\alpha(r_R) = \phi_{RL}(r_R) + \sum \phi_{R'L'}^\alpha(r_R) h_{RL,R'L'}^\alpha$$

Where ϕ is the product of spherical harmonic and the solution $\phi_{vRL}(|r_R|)$ of the radial wave equation inside the sphere centered at R for a certain energy E_{vRL} , which is in principle arbitrary, but in the energy range of interest. The functions ϕ^α are linear combinations of the products ϕ and their energy derivatives ϕ' . The actual choice of how this linear combination is made determines the basis. The matrix h is

given by

$$h^\alpha = C^\alpha - E_v + (\Delta^\alpha)^{1/2} S^\alpha (\Delta^\alpha)^{1/2}$$

Where C^α and Δ^α are the diagonal potential parameter matrices. They depend on the potentials inside the atomic spheres, the representation (α) chosen and on the atomic sphere radii. The S matrix is a structure matrix which depends only on the representation (α) and on the geometrical arrangement of the atomic sites. In term of canonical structure matrix S^0 , S^α is given by

$$S^\alpha = S^0 (1 - \alpha S^\alpha)^{-1}$$

Where α denotes a diagonal matrix, specifying the representation.

In recursion calculations it is practical to work with an orthogonal sparse representation. For this purpose it is advantageous to work in the γ representation. It must be noted, however, that the structure matrix in the γ representation is itself random in an intrinsic way. It is useful therefore to rewrite the Hamiltonian in terms of that in the most localized (or β) representation. The Hamiltonian in the γ representation, which is correct up to second order in $(E - E_v)$, is given by

$$H^2 = E_v + h^\gamma \tag{1}$$

The overlap matrix in this representation is a unit, diagonal matrix and therefore it fulfills the orthogonality condition required for recursion purposes. Expansion of h^γ in terms of the most localized short-ranged h_α is given by

$$h^\gamma = h^\alpha - h^\alpha o h^\alpha - \dots \tag{2}$$

Where the matrix o is diagonal in RL representation and its value is determined by the logarithmic derivative of the function ϕ at the sphere boundary. For a particular choice of $\alpha = \beta$ which are independent of crystal structure given by

$$\beta = \begin{cases} 0.3485 & l = 0 \\ 0.0530 & l = 1 \\ 0.0107 & l = 2 \end{cases}$$

The screened structure constant S^β becomes particularly short ranged with a universal exponential decay for different structures (fcc, bcc, hcp, etc). Due to the exponential behavior of the structure factor, even for s and p bands it is not necessary to consider interactions beyond second nearest neighbors.

If the power series given by (2) is truncated after the first-order term, we obtain a two-centre sparse Hamiltonian. This Hamiltonian is correct up to first order in $(E - E_v)$, and it has been shown that it gives satisfactory band structure description for most solids except those with very broad bands. (Andersen,1985). However, since each term in the second and subsequent terms in the expansion is themselves two-centered and sparse, their inclusion in the recursion method introduces no difficulty. In subsequent sections we will use the first-order, tight-binding two-centre form of the LMTO Hamiltonian given by

$$H^1 = C^\beta + (\Delta^\beta)^{1/2} S^\beta (\Delta^\beta)^{1/2}$$

Again, both the augmented space formalism and recursion method have been described in great detail in earlier work (Andersen,1995; Maan *et al.*,1982). We shall only emphasize those points here which are of relevance to the present work and refer the reader to the articles referenced above for the details.

In the augmented space formalism, we construct a non-random Hamiltonian defined on a new enlarged Hilbert space, which is a direct product of the Hilbert space spanned by the original Hamiltonian basis set and the configuration space which is spanned by the various allowed configuration states of the disordered Hamiltonian. The augmented space theorem (Mookerjee,1973) then relates the configuration averaging to projection onto a particular subspace: the so-called *sum space* (Gray *et al.*, 1976; Mayou *et al.*, 1993 and Julien and Mayon *et al.*,1993). This configuration averaging in the augmented space is exact and does not involve any single-site approximation as in CPA and treats both diagonal and off-diagonal disorder on an equal footing.

The whole process can be summarized in the following basic steps.

(a) Since the probability density $p_i(n_i)$ of random variable n_i associated with the Hamiltonian is a positive semi-definite function and if we assume all its moments to be finite, we may find a self-adjoint operator $M^{(i)}$ in a configuration space $\phi^{(i)}$ such that $p_i(n_i)$ can be expressed as its spectral density.

$$p_i(n_i) = -1/\pi \text{Im} \langle v_0^i | (n_i - M^{(i)})^{-1} | v_0^i \rangle$$

This is the inverse of the well known problem of obtaining a local density of states starting from a self-adjoint Hamiltonian H. If $p_i(n_i)$ can be expressed in continued fraction expansion, then the representation of $M^{(i)}$ is tri-diagonal

matrix with continued fraction coefficients in diagonal and off-diagonal positions.

(2) The averaged quantity $\int f(n_i) p_i(n_i)$ can be shown to be given by the matrix element $\langle v_0^i | \tilde{f}(M^{(i)}) | v_0^i \rangle$ where \tilde{f} is the same functional of $M^{(i)}$ as f was of n_i .

(3) For more than one random variable we define a product of space $\Phi = \Pi^{\otimes \phi^{(i)}}$. This is spanned by states in which the set of variables n_i assumes one of its configurations. The averaged quantity $\langle f \rangle$ is now given by $\langle v_0 | \tilde{f}(M^{(i)}) | v_0 \rangle$

where $|v_0\rangle = \Pi^{\otimes} |v_0\rangle^i$ spans the so-called sum space, which is subspace of Φ . A little algebra will show us that $|v_0\rangle = \Pi_i^{\otimes} (\sum_{\lambda_i} \sqrt{p_{\lambda_i}} |\lambda_i\rangle)$ where $|\lambda_i\rangle$ the eigenstates of $\tilde{M}^{(i)}$ and $\{p_{\lambda_i}\}$ are the associated probability weights.

The calculation of $\langle f \rangle$ thus reduces to calculating a particular matrix element in the augmented space. For electronic structure calculations in a disordered system, f is chosen to the green function $(zI - H(\{n_i\}))^{-1}$ where H is the Hamiltonian of the system and n_i are the random site occupation variables.

An efficient algorithm for calculating diagonal matrix elements of the resolvent or the green function is provided by the recursion method introduced by Haydock and coworkers *et al.*, 1972. Given the starting vector $|\Psi_0\rangle = |i, v_0\rangle$ in augmented space one generates a discrete chain of vectors $|\Psi_i\rangle$ through the following set of equations.

$$\tilde{H} |\Psi_i\rangle = a_i |\Psi_i\rangle + b_{i+1} |\Psi_{i+1}\rangle + b_i |\Psi_{i-1}\rangle$$

$$b_0^2 = \langle \Psi_0 | \Psi_0 \rangle$$

$$b_i^2 = \langle \Psi_i | \tilde{H} | \Psi_{i+1} \rangle$$

$$a_i = \langle \Psi_i | \tilde{H} | \Psi_i \rangle$$

Where \tilde{H} is the operator defined in the augmented space which is constructed by substituting the random site occupation variables $\{n_i\}$ by their associated self-adjoint operator $\{M^{(i)}\}$.

This prescription essentially transforms the effective Hamiltonian H to a trigonal form and thus lead directly to a continued fraction representation for the averaged green function matrix element $\langle \Psi_0 | G | \Psi_0 \rangle = [G_{ii}]_{kv}$. If the algorithm is stop after L steps, L exact levels of the continued fractioned are obtained. The recursion algorithm after L steps contains a contribution only from the central cluster containing $O(L^3)$ sites in the augmented space. For eliminating such a finite-cluster effect L steps of recursion coefficients are appended with a terminator which mimics the asymptotic part of the continued fraction.

Computational Details

The densities of states have been found by the recursion method with the augmented space Hamiltonian. The augmented space map is generated from a real space cluster of 400 atoms. We have generated a sequence of eight couples of continued fraction co-efficient for s, p and d states and the terminating scheme of Lucini and Nex (Lucini *et al.*, 1994) has been used. Regarding the issue of charge self-consistency we have followed the approximate yet accurate and consistent scheme of charge self-consistency proposed by (Andersen *et al.*, 1987). Here the charge neutrality is achieved by exploiting the flexibility in the choice of sizes of Wigner-Seitz spheres of constituents in binary alloys. It involves scaling of the atomic sphere radii of alloy species with the aid of volume derivative correction in such a way that the spheres are approximately charge neutral, a fact discussed in great detail by Kudrnovsky/ and Drchal (Kudrnovsky and Drchal, 1990). Though the augmented space formalism has been recognized as a powerful tool for configuration averaging, its implementation so far has been restricted to model systems. This was because standard recursion cannot deal with the large rank of the augmented space. In particular, the nearest-neighbor map which has to be initially stored for any recursion is too large for storage and manipulations on this map are time consuming. We have reduced this problem to a tractable one by an explicit use of bit manipulation techniques and reduction of the large augmented space to a manageable irreducible subspace on which the recursion could be carried out. As these points have already been described in detail elsewhere (Saha *et al.*, 1995) we will only mention the salient points. The basis vectors defined in the configuration space, carrying information about the occupation variable at each site, are strings of zeros and ones. This allows us to extensively borrow the

Ising computational methodology (Chowdhury *et al.*, 1987) which involves storage of configuration states leads to large-scale saving of disk space while the use of logical operations to describe the action of the augmented space Hamiltonian. The binary word representation of configuration states leads to large scale saving of disk space while the use of logical operations makes the computation faster. The work-load of augmented space recursion is further reduced by exploiting the symmetry of the Hamiltonian. The symmetry of the Hamiltonian arises from that of the underlying lattice and from homogeneity of disorder. It has been shown by Gallagher that if the starting state of recursion belongs to the irreducible representation of the Hamiltonian then the states generated in the process of recursion belong to the same row of the same irreducible representation of the Hamiltonian, so one needs to retain only those states for the purposes of recursion and get the same resolution as with all of them. Since the augmented space recursion retains all the properties of the real space recursion, the confinement of the recursion procedure to the irreducible portion of the Hamiltonian holds good for augmented space recursion also. The basic step in the symmetry procedure is to identify the set of non-equivalent vectors and their weights which can be achieved in augmented space by applying point point group symmetry operations to real space and configuration space by applying point group symmetry operations to real space and configuration space independently. This reduces the rank of the augmented space Hamiltonian drastically, reducing the computer storage and, at the same time, increasing the computer speed.

Results and Discussion

We have applied our methodology, discussed in earlier section to calculating the densities of states of Ni alloys for 10%, 20%, 30%, 40%, 50% and 60% concentration of Cu and 80%, 88%, 90%, 92%, 93%, 94% 95%, 96%, 97%, 98%, 99% concentration of Au per mole. Densities of states of NiCu and NiAu alloys with up and down spin configuration have been put.

Figure 1 to 3 shows the density of states of NiCu alloys with up and down spin configurations. Here, two separated peaks due to Ni and very little deviation due to alloying with Cu are observed. A good deal of variations in the positions and width of the peak and some significant differences in the up and down spin configuration are observed. This trend indicates the on set of the magnetic phase of Cu alloys at some preferred concentrations. There is a broad peak in the density

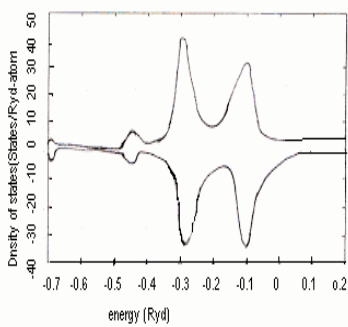
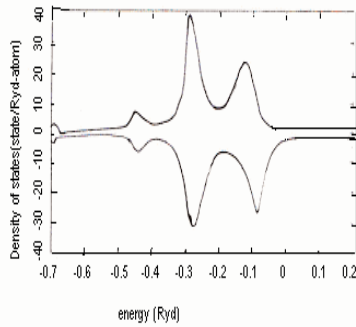
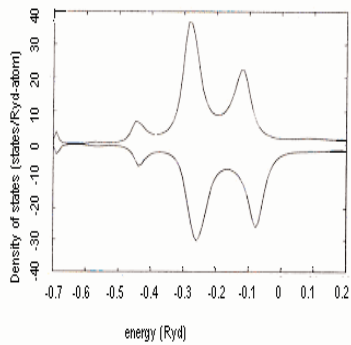


Fig. 1. Density of states for Cu₁₀Ni₉₀(top), Cu₂₀Ni₈₀(middle) and Cu₃₀Ni₇₀(bottom)

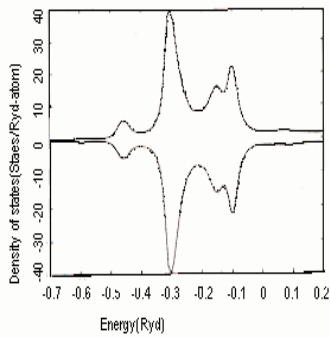
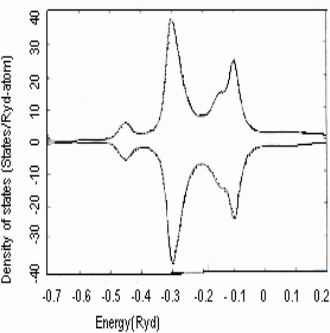
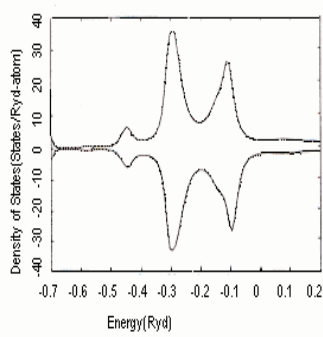


Fig. 2. Density of states for Cu₄₀Ni₆₀ (top), Cu₅₀Ni₅₀ (middle) and Cu₆₀Ni₄₀ (bottom)

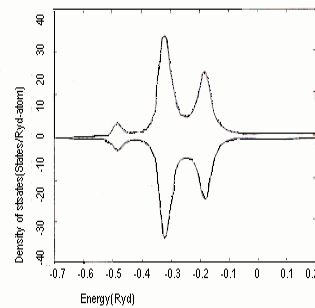
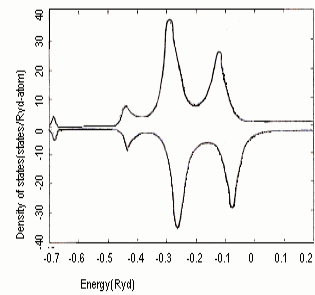


Fig. 3. Density of states for NiNi (top) and CuCu (bottom)

of states and no deviation due to change in concentration are observed. These figures show single prominent peak but with changes in the height and width of the peak due to change in the concentrations.

Figure 4 shows the magnetic moment of NiCu alloy as a function of concentration. At first the magnetic moment of NiCu alloy increases linearly and then decreases sharply. It is observed that the magnetic moment is increased with increasing the concentration of Ni.

Figure 5 shows the plot of Fermi energy as function of magnetic constituents of Ni and Cu. The exact behavior of Fermi

energy depends sensitively on the exact shapes of the density of states and band filling. At first the Fermi energy decreases from a definite value of about -0.94 Rydberg with increasing the concentration of Ni. After reaching to a lowest value of about -0.123 Rydberg, Fermi energy increases with increasing the concentration of Ni. This happens because average number of electrons decreases with decreasing concentration of Ni.

Figure 6 shows the plot of binding energy as function of concentrations of Ni. The binding energy of a electron in an alloy can be calculated from the following relation.

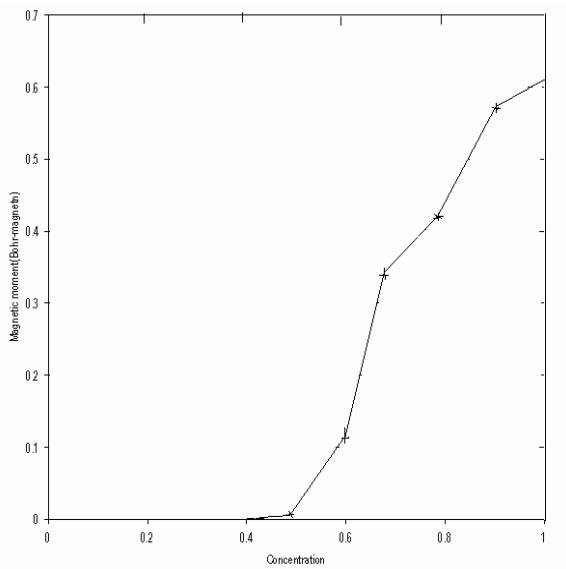


Fig. 4. Magnetic moment at different alloy concentration of CuNi

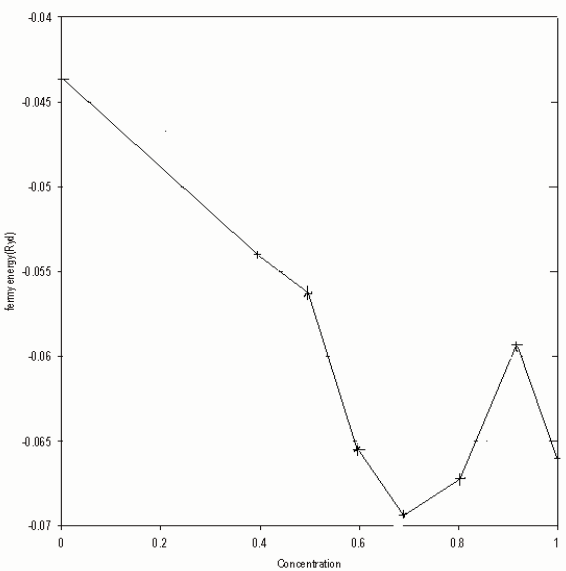


Fig. 5. Fermi energy at different alloy concentration of CuNi

$$\Delta E_{bind} = E_{total}^{alloy} - \{ x E_A^{atom} + (1-x) E_B^{atom} \}$$

where,
$$E_A^{atom} = \int_{-\infty}^{E_F} n(E) E dE$$

And,
$$n(E) \approx n^{\uparrow}(E) + n^{\downarrow}(E)$$

The binding energy of NiCu alloys increases monotonically with increasing the mole fraction of Ni. It means that the

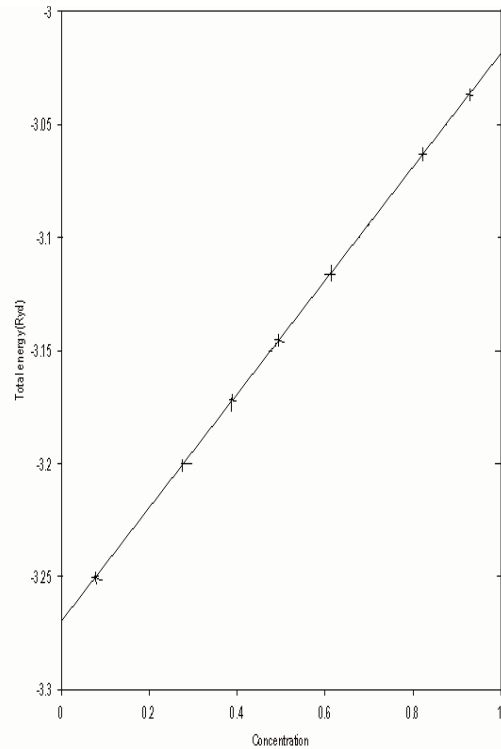


Fig. 6. Total energy at different alloy concentration of CuNi

high concentration of Ni is more stable than the low concentration of Ni in NiCu.

In figures 7 to 10, distinct peaks of Ni-system with very little deviation due to alloying with Au are observed. A single prominent peak is observed. The shifting of peaks at different concentrations is observed for up and down spin cases. The first thing to note is that the s-d bands of Ni and Au do not overlap much.

Consequently in the low concentration regimes of either Ni or Au we have impurity like peaks of the dilute constituents are noticed. The densities of states are hardly spin split and straddle. As concentration of Au increases, the up spin band almost remains fixed, while the down spin band shifts upward in energy.

Figure 11 shows the magnetic moment of NiAu alloy as a function of Ni concentrations. It is observed that the magnetic moment is increased with increasing the concentration of Au and with decreasing the concentration of Ni. It is notable that Au carries negligible magnetic moment. When the concentration of Ni increases, magnetic moment decreases linearly and ends at the point where magnetic moment of AuNi alloy are zero which is actual value.

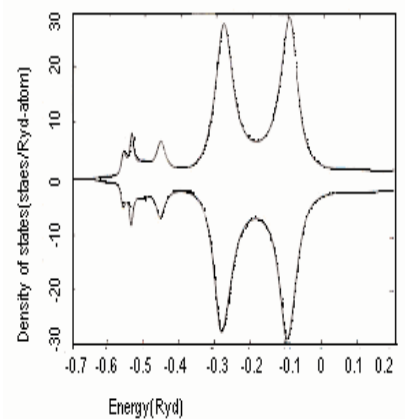
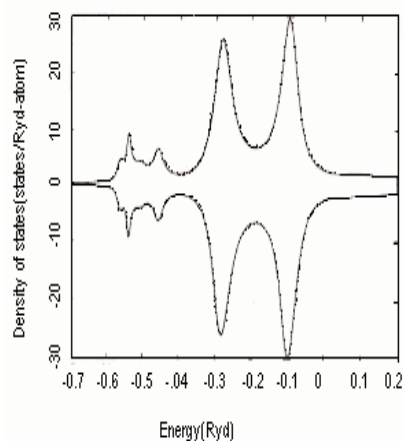
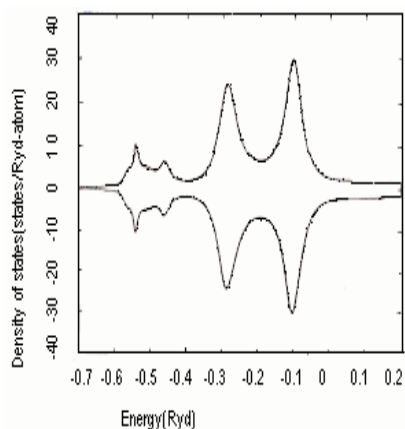


Fig. 7. Density of statea of to NIAu(8812) Middle NiAu (9010) and bottom NIAU (9208)

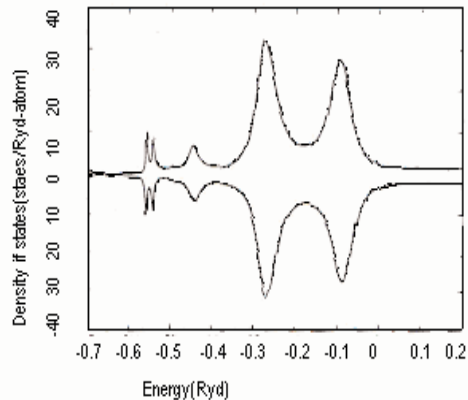
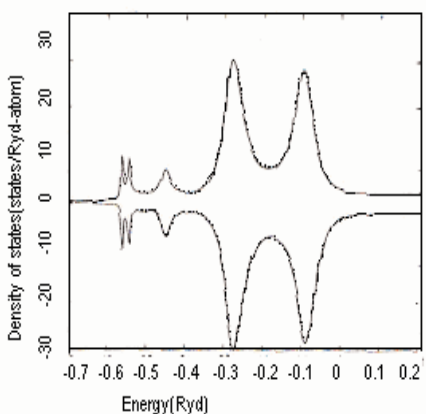
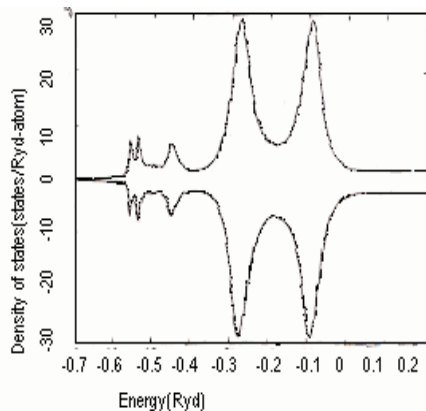


Fig. 8. Density of states for top NiAu (9307), middle NiAu(9406) and bottom NiAu (9505)

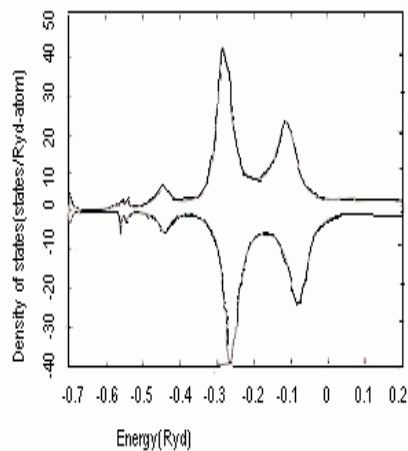
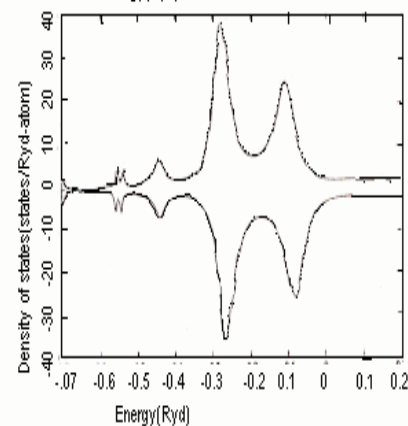
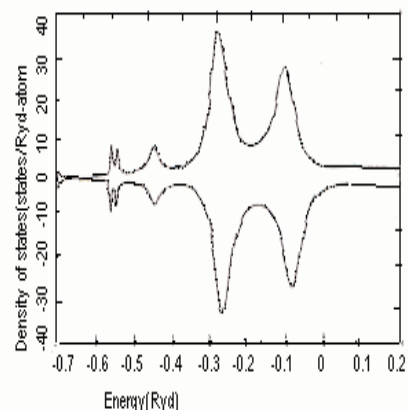


Fig. 9. Density of states for NiAu (9604) top NiAu(9703) middle, NiAu (9802)bottom

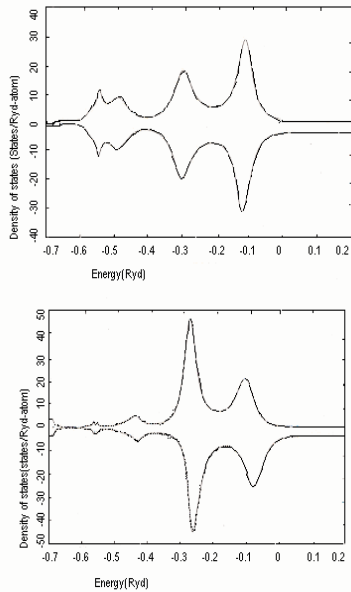


Fig. 10. Density of states for top NiAu(8020) and bottom NiAu(9901)

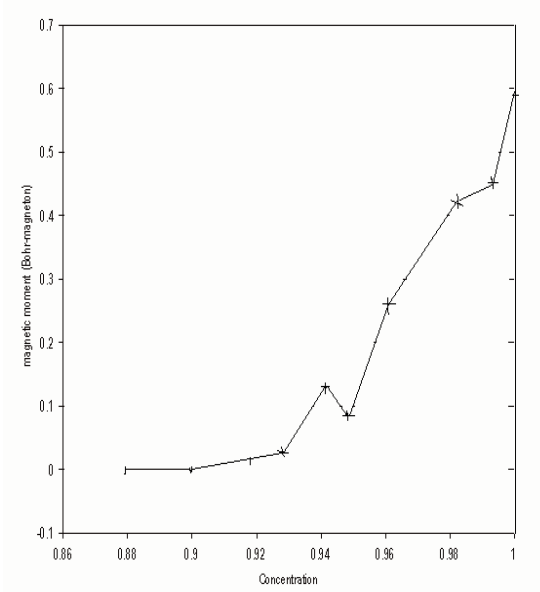


Fig. 11. Magnetic moment at different alloy concentration of AuNi

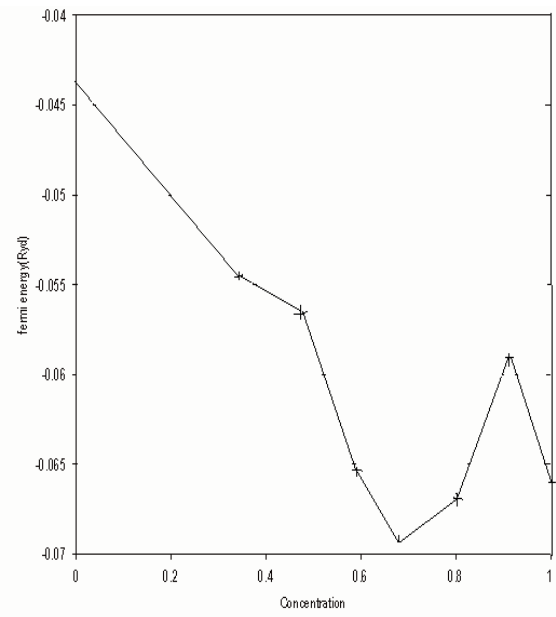


Fig. 12. Fermi energy at different alloy concentration of NiAu

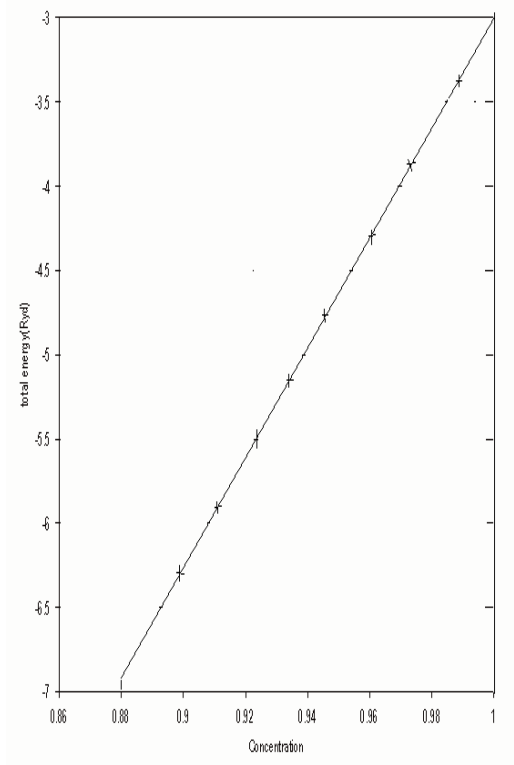


Fig. 13. Total energy at different alloy concentration of AuNi

Figure 12 shows the plot of Fermi energy as a function of concentration of Au and Ni. The exact behavior of the Fermi energy depends sensitively on the exact shapes of the density of states and band filling. Since Au bands lie higher in

energy than Ni, increasing Au concentration leads to upward shift in the Fermi energy.

Figure 13 shows the plot of binding energy as a function of concentrations of Au and Ni. Since Au bands lie higher in energy than Ni, Increasing Au concentration lead also to upward shift in the binding energy. The binding energy of AuNi increases with increasing the concentration of Au. It means that the high concentration of Au is more stable than the low concentration of Au in AuNi.

A set of consistent data have been produced by the efficient, reliable and fast TB-LMTO method on the Ni-based alloys of Au and Cu. The all have peaks in the density of states and these are consistent with the previous calculations (Bratkovsky *et al.*, 1993).

Conclusion

The electronic structure of NiCu and AuNi alloys using fully self-consistent first principles electronic structure technique have been calculated and obtained results agrees reasonably-well with the experimental results (Bratkovsky *et al.*, 1993). This clearly shows that ASR coupled with TB-LMTO is a powerful technique in describing electronic structure of binary alloys. Results clearly show the flaws in the theoretical results based upon model calculations. The band structure can be computed from here. These studies are going to be helpful for experimentalist and metallurgists, who would design materials and alloys with specific properties.

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Received : August 13, 2008;

Accepted : February 11, 2009