Electronic structure of chromium-aluminium alloys

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The electronic structure of Cr-Al alloys has been studied by using the charge self-consistent Korringa-Kohn-Rostoker Coherent Potential Approximation method. Results for density of states are presented and found to be in very good agreement with reflected X-ray photo spectra results. It has been found that half width of density of states band of these alloys increases approximately 5 per cent at 85 atomic percentage of Cr with respect to 95 and 75 percentage of Cr, which explains the change in shape and half width of experimental X-ray photo spectra results.

Keywords: Electronic structure, Chromium-aluminium alloys, Alloys

1 Introduction

During the past two decades, the Korringa-Kohn-Rostoker Coherent Potential Approximation (KKR-CPA), has been very successful in understanding the electronic structure of disordered alloy. In the present work, the electronic structure of disordered paramagnetic Cr-Al alloys by using the charge self-consistent KKR-CPA has been studied. This system is chosen because this is very important for bcc alloy system. CrₓAlᵧ alloy system forms bcc solid solution for 1 ≥ X ≥ 74.5. Some important experimental results of X-ray photo spectra (XPS) and X-Ray emission spectra (XES) of the valence band on concentration X=1.0, 0.95, 0.85, 0.80 and 0.75 are available on Cr-Al alloys. The results for the density of states which is the basic quantity needed to explain the various experimental results, have been presented.

2 Charge Self-consistent KKR-CPA

The charge self-consistent KKR-CPA method has been discussed in detail earlier. Let us consider a binary alloy AₓBᵧ where X and Y are atomic concentrations. The basic quantity of interest is the ensemble-averaged Green’s function of the alloy. The Green’s function for a particular configuration of the alloy can be written as :

\[ G(E,\vec{r},\vec{r}') = \sum_{LL'} Z^L_n(E,\vec{r}_n) T^{LL'}_{nm} (\chi) Z^L_m(E,\vec{r}_m) \]

\[ - \delta_{nm} \sum_L Z^L_n(E,\vec{r}_n) J^L_n(E,\vec{r}_n) \]  

where \( \vec{r} \) and \( \vec{r}' \) are within \( n^{th} \) and \( m^{th} \) muffin-tin spheres and the wave functions \( Z^L_{n(m)}(E,\vec{r}_{n(m)}) \) are, respectively, the regular and irregular solutions of the Schroedinger equation for the single muffin-tin potential centered at \( \vec{r}_n \) and the \( T^{nm} \) are path operators. The ensemble-average of Eq. (1) is related to the ensemble-average of the path operators, which is determined by invoking the CPA. The CPA condition, that the average scattering from each site must be zero, can be expressed as:

\[ [T^{-1}_C]_{LL'} = [x,t_A^{-1} + y,t_B^{-1} + (t_A^{-1} - t_B^{-1})T^C_{00}(t_A^{-1} - t_B^{-1})]_{LL'} \]  

where \( t_{A(B)} \) denotes on-the-energy-shell matrix element of the \( t \)-matrix of an isolated A(B) atom and C is used to label quantities for the CPA medium. The path operator matrix is given by:

\[ [T^C_{00}]_{LL'} = \frac{\Omega}{(2\pi)^3} \int \left[ \left[ t_C^{-1} - B_\kappa (\chi) \right]^{-1} \right]_{LL'} d\vec{K} \]  

where \( \Omega \) is the unit cell volume. \( T^C_{00} \) involves a complicated Brillouin zone integration. Though \( B_\kappa (\chi) \) is an off-diagonal matrix, for cubic symmetry the integral reduces to a diagonal matrix for 1≤2. For full charge self-consistency, the charge densities in A and B cells are needed. These can be obtained, once the restricted site averages of the Green’s function < \( G(E,\vec{r},\vec{r}') >_{A(B)} \) as:
\[ \rho_{A(B)}(\vec{r}) = -\left(\frac{1}{\pi}\right) \int_{-\infty}^{\infty} \text{Im} <G(E, \vec{r}, \vec{r}') >_{A(B)} dE \quad \ldots (4) \]

where \( \rho_{A(B)} \) denotes the charge density associated with an A (B) cell.

The component density of states for the A and B atoms can be expressed as:

\[ \rho_{A(B)}(E) = -\left(\frac{1}{\pi}\right) \text{Im} \int_{\Omega} <G(E, \vec{r}, \vec{r}') >_{A(B)} d\vec{r} \]

or

\[ \rho_{A(B)}(E) = -\left(\frac{1}{\pi}\right) \text{Im} tr \left[ F^{A(B)} D_{A(B)} T_{00}^{C} \right]_{L,L} \quad \ldots (5) \]

where \( tr \) denotes the trace in L-space. Since Eq. (5) is diagonal in L-space, it allows L decomposed symmetry components (s,p,t_\| and e_\|) of \( \rho_{A(B)}(E) \) in the alloy.

The average density of states for the alloy is calculated as:

\[ \rho(E) = x \rho_A(E) + y \rho_B(E) \]

### 3 Computational Details

The charge self-consistent KKR-CPA method is applied to the CrXAlY alloy for different concentrations of Cr (X=1.0, 0.95, 0.85 and 0.75). This alloy has bcc structure and their lattice constants are presented in Table 1.

For the charge self-consistent KKR-CPA, we start with atomic charge densities \( (\rho_{A}^\text{in}, \rho_{B}^\text{in}) \) for Cr and Al, and calculate the potentials \( (V_{A}^\text{in}, V_{B}^\text{in}) \) using the local density approximation. The \( t_{\alpha}^{-1}(x) \) and \( t_{\beta}^{-1}(x) \) are then computed for the input potentials \( (V_{A}^\text{in}, V_{B}^\text{in}) \). We have used the tetrahedron method using 858 \( \bar{K} \) points in the irreducible part of the Brillouin Zone for the calculation of path operator \( (T_{00}^{C}) \). After solving the KKR-CPA, Eq. (2) iteratively, the new charge densities \( (\rho_{A}^\text{out}, \rho_{B}^\text{out}) \) are obtained by Eq. (4). The new potentials \( (V_{A}^\text{out}, V_{B}^\text{out}) \) in the alloy are then calculated.The whole calculation is repeated, until the difference of old and new charge densities is with in a certain tolerance (integrated rms difference between input and output charge densities \( \leq 0.0001 \) electrons). Fermi energy is calculated by generalized Lioyds formula which does not give unphysical jumps in the integrated density of states.

To speed up the calculations, the complex energy method and mixing scheme in both CPA and the charge self-consistency loops have been used to calculate the charge densities and potentials.

### 4 Results and Discussion

The charge self-consistent KKR-CPA method is applied for calculating the electronic structure of paramagnetic bcc CrXAlY alloys. The charge self-consistent potential, charge densities, component density of states and density of states of CrXAlY alloys for concentrations X = 0.95, 0.85 and 0.75 are calculated. Component density of states, density of states and density of states at Fermi energy for above concentrations are shown in Figs 1-6. These results can be used directly for calculating electronic structure (Fermi surface, band structure, conductivity, optical properties and transport properties) of the alloys. Calculated density of states are compared with

**Table 1 — Lattice constants of CrXAlY alloys**

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Cr concentration (X)</th>
<th>Lattice constants (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.00</td>
<td>5.453</td>
</tr>
<tr>
<td>2</td>
<td>0.95</td>
<td>5.484</td>
</tr>
<tr>
<td>3</td>
<td>0.85</td>
<td>5.508</td>
</tr>
<tr>
<td>4</td>
<td>0.75</td>
<td>5.553</td>
</tr>
</tbody>
</table>

![Fig. 1 — Component density of states of Cr (solid curve) and Al (broken curve) in Cr_{0.85}Al_{0.15}](image-url)
experimental measured X-Ray photo spectra (XPS) of \( \text{Cr}_x\text{Al}_y \) alloys at concentration \( x=0.95, 0.85 \) and 0.75.

Fig. 2 — Component density of states of Cr (solid curve) and Al (broken curve) in \( \text{Cr}_{0.85}\text{Al}_{0.15} \).

Fig. 3 — Component density of states of Cr (solid curve) and Al (broken curve) in \( \text{Cr}_{0.75}\text{Al}_{0.25} \).

Fig. 4 — Average density of states by using charge self-consistent KKR-CPA method (solid curve) and experimental X-ray photo spectra results (broken curve) for \( \text{Cr}_{0.95}\text{Al}_{0.05} \).
In Figs 1-3, the component density of states of Cr and Al in CrXAlY alloys for concentration X=0.95, 0.85 and 0.75 respectively are shown. These results can be used in the analysis and calculations of electronic structure of these alloys. The component density of states can be compared with experimental results of soft X-ray (emission and absorption) spectra. Therefore, these results will be very important for researchers.

In Fig. 4, the comparison of the charge self-consistent KKR-CPA density of states (theoretical results) with available results of X-Ray photo spectra (XPS) for Cr0.95Al0.05 alloy is shown. The structures (the position of peaks) in theoretical results are well reflected in X-ray photo spectra (XPS) results. The theoretical half-width of density of states (DOS) curve below Fermi energy is 2.20 Rydberg approximately. It has been found that results obtained are in good agreement with experimental results.

In Fig. 5, the comparison of the charge self-consistent KKR-CPA density of states (theoretical results) with available results of X-ray photo spectra (XPS) for Cr0.85Al0.15 alloy is shown. The structures in the theoretical results are very well reflected in X-ray photo spectra (XPS) results. The theoretical half-width of density of states (DOS) curve below Fermi energy is 2.31 Rydberg approximately. It is noticed that the half-width of the band increases about 5% of the Cr0.95Al0.05 alloy, which is quite satisfactory with XPS experimental results. Thus it has been found that theoretical results are in very good agreement with experimental results.

In Fig. 6, the comparison of the charge self-consistent KKR-CPA density of states (theoretical results) with available results of X-ray photo spectra (XPS) for Cr0.75Al0.25 alloy is shown. The structures in the theoretical results are in very good agreement with reflected X-ray photo spectra (XPS) results. The theoretical half-width of density of states (DOS) curve below Fermi energy is 2.20 Rydberg approximately. It is observed that the half-width of the theoretical band decreases about 5 per cent with respect to Cr0.85Al0.15 alloy. Thus, it has been found that half-width of the DOS band changes approximate 5% at 85 atomic percentage of Cr. It is less for 95 and 75 atomic percentage of Cr, as reported in XPS results. Therefore, the results of calculated KKR-CPA density of states (DOS) are in very good agreement with XPS experimental results.
5 Conclusions

The charge self-consistent KKR-CPA method to calculate the electronic structure of Cr$_x$Al$_{1-x}$ disordered alloy system is applied in this study. Component density of states and density of states for concentrations $X=0.95$, 0.85 and 0.75 by using the charge self-consistent KKR-CPA method are presented. It is found that charge-self consistent KKR-CPA density of states for different concentrations of alloy is in very good agreement with reflected X-ray photo spectra (XPS) results. It is also found that half-width of density of states band of these alloys increases approximately 5% at 85 atomic percentages of Cr with respect to 95 and 75 per cent of Cr and agrees with the change in shape and half-width of experimental XPS results.

References


