

Electronic band structure of disordered Fe₃Mn

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The multiple-scattering theory is applied for determining of electronic spectrum of Fe₃Mn alloy for long-range order parameters $\eta_1 = 1$ (ordered states) and $\eta_2 = 0.75$ (disordered state). The essential difference of disordered alloy from ordered alloy is in existence local states. These local states possess *d* - symmetry and almost not depend on wave vector. Imaginary paths of local energies are large so that they overlap with each other and with the main component bands. Thus disordering of atoms in Fe₃Mn alloy is possible with appearance energy-bands of iron and manganese in another sublattices.

1. INTRODUCTION

Most of alloys are disordered systems. Variety of optical, magnetic, mechanical and another properties of disordered systems stimulates intensive development of physical research methods for study of phenomenon's, which depend on the order parameter. This variety of properties has been found to be governed by the particulars of electronic structure. Therefore it is necessary to examine the real electronic structure and properties, which depend on the electronic structure of the concrete material.

2. METHOD

Considerable progress has been achieved in the theoretical study of the electronic structure of disordered metallic alloys. This was enabled by combination of single-site approximation line coherent-potential approximation and the average-T-matrix approximation extensively studied using simple tight-binding model, with the well established Kohn-Korringa-Rostoker method [1,2] concerned with more realistic muffin-tin potentials. Unfortunately both methods require relatively great numerical effort, in particular, the self-consistent coherent-potential approximation. However we consider that average-T-matrix approximation has

several advantage. The application of the multiple-scattering theory with the muffin-tin potential to disordered FeCo was demonstrated in [3]. In this section we follow directly these ideas.

Let's consider a substitutional-binary-alloy with the complex Ising lattice. Let $\mathbf{R}_{pi} = \mathbf{R}_p + \boldsymbol{\tau}_i$ be vectors of the lattice sites, where \mathbf{R}_p - vector of the direct lattice and $\boldsymbol{\tau}_i$ - vector in the direct primitive cell. Effective potential has the usual representation of random by distributed scatterers

$$V(\mathbf{r}) = \sum_{sip} C_s(\mathbf{R}_{pi}) V_s(\mathbf{r} - \mathbf{R}_{pi}), \quad (1)$$

as given by a sum of cell potentials $V_s(\mathbf{r} - \mathbf{R}_{pi})$, where *s* - type of atom A or B. $C_s(\mathbf{R}_{pi})$ is equal 0 or 1 depending on whether an atom of type A or B occupies the site \mathbf{R}_{pi} .

For a given configuration the Green's function may be defined by

$$G = G_0 + G_0 T G_0 \quad (2)$$

where G_0 - free electron Green's function. The T-matrix is defined as solution of the equation

$$T = V + V G_0 T \quad (3)$$

By iterating Eq.(3) can be rewritten

$$T = \sum_{sip} C_s(\mathbf{R}_{pi}) t_{spi} \quad (4)$$

$$+ \sum_{sp} \sum_{s'i'p' \neq p} C_s(\mathbf{R}_{pi}) t_{spi} G_0 t_{s'p'i'} C_{s'}(\mathbf{R}_{p'i'}) + \dots$$

where

$$t_{spi} \equiv V_s(\mathbf{r}-\mathbf{R}_{pi}) + V_s(\mathbf{r}-\mathbf{R}_{pi}) G_0 C_s(\mathbf{R}_{pi}) t_{spi} \quad (5)$$

site's t-matrix.

Eq. (2) can be rewritten in l - representation

$$G(\mathbf{r}, \mathbf{r}') = G_0(\mathbf{r}, \mathbf{r}') + \sum_{spL} \sum_{s'i'p'L'} (-i\sqrt{\varepsilon})$$

$$\times h_l(\sqrt{\varepsilon} |\mathbf{r} - \mathbf{R}_{pi}|) Y_L(\mathbf{r} - \mathbf{R}_{pi}) \tau_{spis'p'i'}^{LL'} \quad (6)$$

$$\times h_l(\sqrt{\varepsilon} |\mathbf{r}' - \mathbf{R}_{p'i'}|) Y_L(\mathbf{r}' - \mathbf{R}_{p'i'}) (-i\sqrt{\varepsilon}),$$

where h_l - Hankel function,

$$\tau_{spis'p'i'}^{LL'} = C_s(\mathbf{R}_{pi}) t_{spi}^L \delta_{pp'} \delta_{ii'} \delta_{ss'} \delta_{LL'}$$

$$\times \sum_{L''s''i''p'' \neq p} C_s(\mathbf{R}_{pi}) t_{spi}^L g_{pip''i''}^{LL''} \tau_{s''p''i''s'p'i'}^{L''L'} \quad (7)$$

which can be averaged on every kind configurations without any correlations.

$$\langle \tau_{spis'p'i'}^{LL'} \rangle = n_{is} \langle t_{is}^L \rangle \delta_{ii'} \delta_{ss'} \delta_{LL'} \delta_{pp'}$$

$$+ \sum_{L''s''i''p'' \neq p} n_{is} g_{pip''i''}^{LL''} \langle t_{is}^L \rangle \langle \tau_{s''p''i''s'p'i'}^{L''L'} \rangle \quad (8)$$

By using the Fourier transformation of Eq. (8)

$$\tau_{is'i's'}^{LL'}(\mathbf{k}) = n_{is} n_{is'} \{ \delta_{ii'} \delta_{ss'} \delta_{LL'} n_{is} \langle t_{is}^L \rangle^{-1}$$

$$- n_{is} g_{is'i's'}^{LL'}(\mathbf{k}) n_{i's'} \}^{-1} \quad (9)$$

we have finally

$$\| \delta_{ii'} \delta_{ss'} \delta_{LL'} n_{is} \langle t_{is}^L \rangle^{-1} - n_{is} g_{is'i's'}^{LL'}(\mathbf{k}) n_{i's'} \| = 0 \quad (10)$$

- secular equation for finding of the alloy energy spectrum. In equation (10) $n_{is} = \langle C_s(\mathbf{R}_{pi}) \rangle = c_s \pm \gamma \eta$ [4], $g_{is'i's'}^{LL'} = A_{ii'}^{LL'} + i\sqrt{\varepsilon} \delta_{ii'} \delta_{LL'}$, $\langle t_{is}^L \rangle^{-1} = \sqrt{\varepsilon} \times (\text{ctg} \delta_{is}^L - i)$, η - long-range-order parameter, c_s - concentration of s-type atoms, $A_{ii'}^{LL'}$ - structure constants [5], δ_{is}^L - l-partial phase shift [6].

3. RESULTS OF CALCULATIONS AND DISCUSSION

To calculate the energy-band $\varepsilon = E(\mathbf{k}) + i\Gamma(\mathbf{k})$ of disordered Fe₃Mn the method applied in [3,6] was used. Electronic structure calculation of ordered Fe₃Mn with $\eta = 1$ was made using the same programs, which were used to calculate disordered

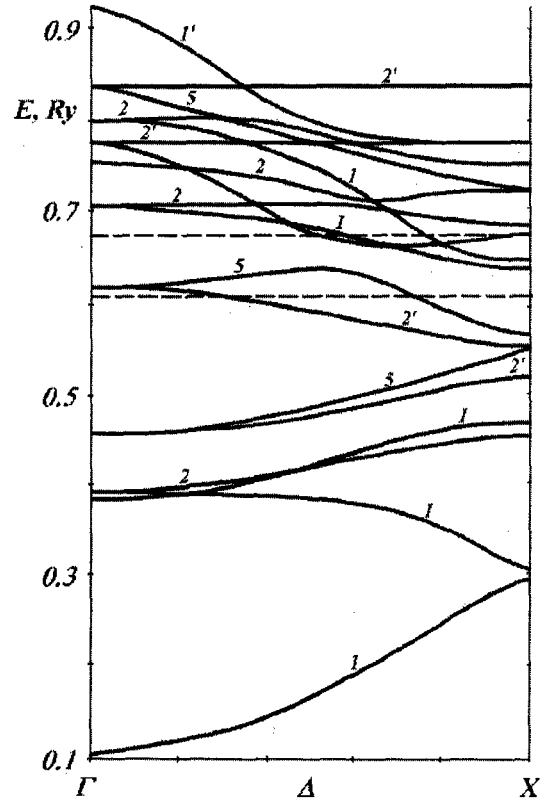


Figure 1. Electronic band structure $E(\mathbf{k})$ of disordered Fe₃Mn alloy with $\eta = 0.75$ along Δ -direction of symmetry.

Table 1.

Energy values $\varepsilon = E(\mathbf{k}) + i\Gamma(\mathbf{k})$ in Ry for Γ and X points of high symmetry. All $\Gamma(\mathbf{k}) = 0$ for ordered Fe_3Mn with $\eta = 1$.

η	1		0.75	
\mathbf{k}	$E(\mathbf{k})$	$E(\mathbf{k})$	$E(\mathbf{k})$	$\Gamma(\mathbf{k})$
Γ_1	0.104	0.105	0.0000	
Γ_1	0.384	0.386	0.0000	
Γ_{12}	0.390	0.391	0.0000	
$\Gamma_{25'}$	0.457	0.458	0.0001	
$\Gamma_{25'}$	0.621	0.620	0.0039	
Γ_{12}	0.708	0.706	0.0040	
Γ_1	0.755	0.754	0.0035	
$\Gamma_{25'}$	0.777	0.775	0.0035	
$X_{4'}$	0.297	0.298	0.0001	
X_1	0.310	0.311	0.0001	
X_2	0.457	0.458	0.0002	
X_1	0.472	0.473	0.0002	
$X_{2'}$	0.524	0.526	0.0002	
X_5	0.548	0.549	0.0003	
X_3	0.549	0.548	0.0002	
X_5	0.564	0.563	0.0003	
		0.619	0.0382	
		0.672	0.0601	

Fe_3Mn with $\eta = 0.75$. The lattice spacing was supposed in variable and equal 6.7994 a.u. The energy bands resulting from this calculations are shown along Δ - direction of symmetry in Fig.1. The shape of the main spectrum curves $E(\mathbf{k})$ has almost

not changed with disordering of atoms. Our present calculated energy values are listed in Table 1 for Γ and X points of high symmetry. Imaginary path $\Gamma(\mathbf{k})$ of electronic spectrum in disordered Fe_3Mn is not equal naught. Small values of imaginary path indicate that these electronic states $E(\mathbf{k})$ have a large life time. The essential difference of disordered alloy from ordered alloy is in existence local states. Dashed line are these local states in Fig.1. The local states $E(\mathbf{k})$ possess d - symmetry and almost not depend on wave vector. Imaginary path of local energies are large so that they overlap with each other and with the main component bands (see tow east lines in Table 1).

Thus disordering of atoms in Fe_3Mn alloy is possible with appearance energy-bands of iron and manganese in another sublattices.

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