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MAGNETIC AND ELECTRONIC PROPERTIES OF CoTi ALLOYS

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Abstract: The influence of the local environment on the electronic and magnetic properties of Co-Ti systems is studied by *ab-initio* spin-polarized tight binding LMTO method. We have performed the self-consistent band calculations for Co and Ti atoms distributed in the cubic $L2_1$ and hexagonal type structure. Using the $L2_1$ type structure we have studied the effect of alloying between Co and Ti layers. The *ab-initio* calculations indicated that the magnetic moment on Co atom decreased about 50% near the Ti layers.

1. INTRODUCTION

The interesting magnetic and electronic properties of Co-Ti systems (bulk and multilayers) have been studied intensively experimentally and theoretically in the last years [1-4]. CoTi alloy which crystallizes in the bcc type structure is non-magnetic. Magnetic moment of Co in the hexagonal structure is $m = 1.63\ \mu_B$. The value of the magnetic moment on Co atom depends strongly on the type of the local environment. In this paper we present the magnetic and electronic properties of Co-Ti systems in which Co and Ti atoms are distributed in the hexagonal and $L2_1$ type structures. Particularly the $L2_1$ structure gives the possibility to study the effect of alloying between Co and Ti layers. In Section 2 we present the method of calculation and the results are presented in Section 3.

2. METHOD OF CALCULATIONS

The band structure and magnetic moments were calculated by spin-polarized self-consistent Tight Binding Linear Muffin Tin Orbital (TB LMTO) method [5-7] in Atomic Sphere Approximation (ASA) for the experimental lattice parameters. We applied the scalar-relativistic approximation for band electrons and the fully-relativistic treatment of the frozen core electrons. The values of the atomic sphere radii were taken in such a way that the sum of all atomic sphere volumes was equal to the volume of the unit cell and the values of the atomic potentials at the sphere boundaries were similar. The exchange correlation potential was assumed in the form proposed by von Barth and Hedin [8] and non-local corrections were also applied [9]. In the band calculations the initial atomic configurations were taken according to the Periodic Table of Elements. In the band calculations we used more then 270-k points in the irreducible wedge of the Brillouin zone and the number of k-points depended on the type of the structure.

The Co and Ti atoms were distributed in the cubic $L2_1$ (CoTi) and hexagonal ($Co_{0.625}Ti_{0.375}$) structures. The cubic $L2_1$ type structure which consists of four interpenetrating fcc sublattices with the origins at (0, 0, 0), (0.5, 0.5, 0.5), (0.25, 0.25, 0.25) and (0.75, 0.75, 0.75). In order to study the effect of local environment we replace each fcc sublattice by four simple cubic (sc) sublattices . In this way we have a unit cell of 16 atoms and four types of atoms can be distributed in each layers. In this type of structure we studied the effect of alloying between Co and Ti layers.

We consider also the effect of the tetragonal distortion in the hexagonal type structure for $Co_{0.625}Ti_{0.375}$ (Co_5Ti_3) system. We assumed that the volume of the unit cell is the same during the distortion and we changed the values of a and c lattice parameters.

3. RESULTS

3. 1. Effect of alloying in CoTi alloy in $L2_1$-type structure

The effect of alloying in CoTi alloy we study using the unit cell, which consists of four layers, and in each layer there are four positions for Co and Ti atoms. We have performed the spin-polarized band calculations for CoTi alloys in the five different configurations listed in Table I.

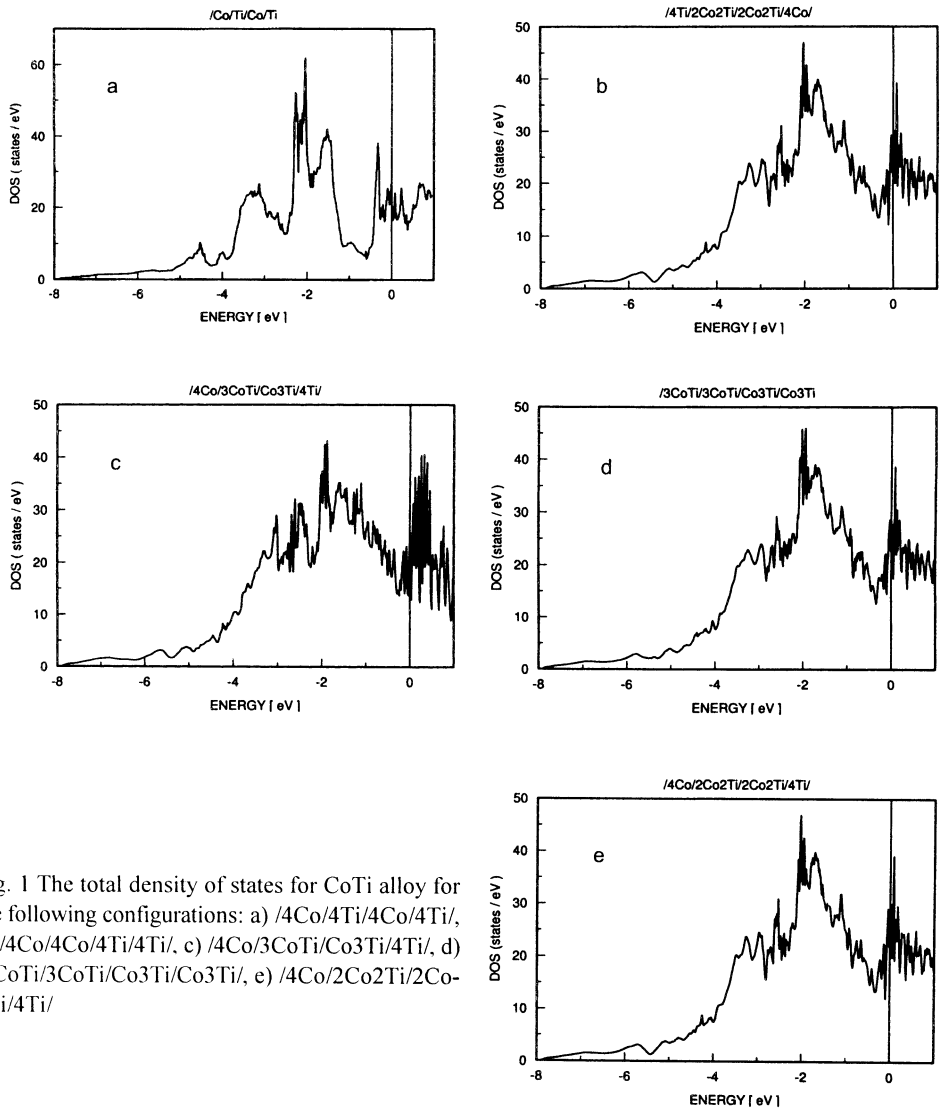

Fig. 1 The total density of states for CoTi alloy for the following configurations: a) /4Co/4Ti/4Co/4Ti/, b) /4Co/4Co/4Ti/4Ti/, c) /4Co/3CoTi/Co3Ti/4Ti/, d) /3CoTi/3CoTi/Co3Ti/Co3Ti/, e) /4Co/2Co2Ti/2Co-2Ti/4Ti/

In Fig. 1a we present the DOS for ordered CoTi alloy (/4Co/4Ti/4Co/4Ti/). This system is paramagnetic. The total density of states has a deep valley below the Fermi level. In the DOS there are several sharp peaks. In the case when four layers are occupied by Co and the next four by Ti we have got also paramagnetic system.

Table I. The values of the magnetic moments in Co_8Ti_8 alloys for the different distributions of Co and Ti atoms in the $L2_1$ type structure

Configuration	Total magnetic moment μ_B
/ 4Co / 3CoTi / Co3Ti / 4Ti /	1.83
/3CoTi / Co3Ti / 3CoTi /Co3Ti /	1.35
/ 4Co / 4Ti / 4Co/ 4Ti /	0.0
/ 4Co / 4Co / 4Ti / 4Ti /	0.0
/4Co / 2Co2Ti / 2Co2Ti / 4Ti /	1.56

In the next configurations we have studied the effect of alloying between Co and Ti layers. The total densities of states for five given configurations are plotted in Fig. 1 (a-e). We observe the change of the shape the density of states. The chemical disorder gives many peaks in the DOS. The values of the total magnetic moments are listed in Table I. The general shape of the density of states is similar for all three configurations. The main contribution below the Fermi level is coming from the cobalt atoms.

3. 2. Tetragonal distortion in the hexagonal $Co_{0.625}Ti_{0.375}$ alloy

The magnetic moment of the Co in the hexagonal structure (c/a = 1.623) is $m = 1.63\mu_B$. We considered the hexagonal supercell consisted of 5 Co and 3 Ti layers that corresponded to $Co_{0.625}Ti_{0.375}$ alloy. In this model each 5 Co layers were separated by 3 Ti layers (.../5Co/3Ti/5Co/...). We change the lattice parameter a from 2.54 Å to 2.49 Å and the value of c parameter was chosen so as to keep the volume of the unit cell constant. In Figure 2 we plotted

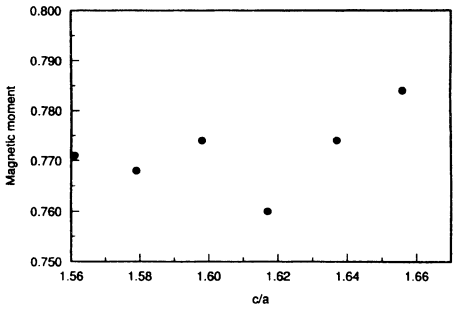

Fig. 2. The dependence of total magnetic moment in $Co_{0.625}Ti_{0.375}$ on c/a in the hexagonal structure

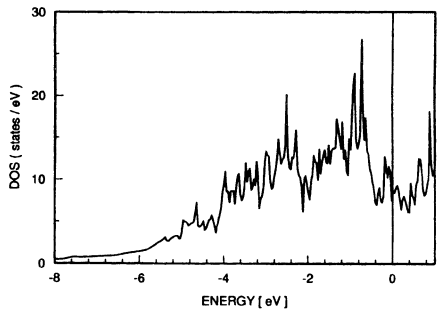

Fig. 3. The total density of states of $Co_{0.625}Ti_{0.375}$ for c = 1.6173. The Fermi level is located at E = 0 eV

the change of the total magnetic moment versus c/a. The total energy of the system has a minimum for c/a = 1.6173. The values of local magnetic moments in each layer are /Co(1.55-1.56 μ_B)/ Co(0.75-0.78 μ_B)/ Ti (-0.06 μ_B)/ Ti(0.11μ_B) / Ti(-0.06μ_B) /Co (0.75-0.78 μ_B) /Co (1.55-156 μ_B). We observed that the magnetic moment on Co near titanium layer decreased almost two times. The local magnetic moment on Ti is small but it is negative near cobalt layer and positive when Ti layer is surrounded by Ti layers from both sides. The similar tendency we observed also for CoTi system with bcc and fcc type structures. The total density of states for $Co_{0.625}Ti_{0.375}$ for c/a = 1.6173 is plotted in Fig. 3.

4. CONCLUSIONS

In this work we presented the influence of the local environment on the electronic and magnetic properties of CoTi and $Co_{0.625}Ti_{0.375}$ alloys. In the first case we have shown how the effect of alloying change the magnetic moment of Co atom. The second example had shown that the value of the magnetic moment of Co did not change drastically during the tetragonal distortion in the hexagonal structure.

The spin-polarized band calculations indicated that the value of the magnetic moment on Co decreased about 50% near titanium layers.

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