Electronic structure and magnetic properties of SmCo$_{7-x}$Ti$_x$

ZHANG Changwen$^1$, LI Hua$^1$, DONG Jianmin$^1$, GUO Yongquan$^2$ & LI Wei$^2$

1. School of Physics and Microelectronics, Shandong University, Jinan 250100, China;
2. Institute of Functional Materials, Central Iron and Steel Research Institute, Beijing 100081, China

Correspondence should be addressed to Li Hua (email: huali@sdu.edu.cn)

Received September 20, 2004; accepted January 31, 2005

Abstract  Electronic structure of SmCo$_{7-x}$Ti$_x$ alloy has been studied by means of the spin-polarized MS-X$\alpha$ method. It is shown that a few of electrons are transferred to Sm(5d) orbital due to orbital hybridization between Sm and Co atoms. The exchange interaction between 5d-3d electrons is stronger, which is the main reason resulting in the long-range ferromagnetic order between Co and Sm atoms. The Curie temperature of SmCo$_{7-x}$Ti$_x$ is generally lower than that of pure Co metal, which may be explained by the weaker average of coupling strength between Co sites due to some negative exchange couplings occurring mainly at 2e site. The calculated results for the Sm$_5$Co$_{28}$Ti$_6$ cluster may lead to a better understanding of why SmCo$_{7-x}$Ti$_x$ is stable phase. Since the negative interaction of 2e sites weakens and the bonding at $E_F$ strengthens with increasing Ti concentration, which result in the decrease in the free energy of the alloy, the stable ferromagnetic order forms inside SmCo$_{7-x}$Ti$_x$. Considering the localization of 4f states and 5d moment arising from the orbital hybridization, the calculated moment is 9.47$\mu_B$ per formula unit that is in agreement with experiments.

Keywords: electronic structure, spin polarization, atomic magnetic moment, exchange coupling, Curie temperature.

Interest has recently been focused on the Sm-Co intermetallic alloys with the TbCu$_7$-type structure due to their potential applications as novel high temperature permanent magnetic materials$^{[1-3]}$. However, the pure binary SmCo$_7$ alloy with the TbCu$_7$-type structure does not exist stably at room temperature and a third metal element is necessary to replace a proportion of Co atom in order to stabilize the Sm(Co, $M$)$_7$ ($M$ = Zr, Ti, Si, etc.)$^{[4-9]}$ with the TbCu$_7$-type structure. There are three kinds of exchange coupling in Sm-Co-based alloys, i.e. Co-Co, Sm-Co and Sm-Sm couplings. From superfine field experiments, it is found that the exchange coupling between Sm-Sm atoms is negligibly small compared with the first two couplings. In general, the exchange coupling between Sm(4f)-Co(3d) has the same order of magnitude as that of the Co(3d)-Co(3d), but the
latter holds the upper hand over the former. Some authors\cite{10} have inferred that polarization effect of conductive electrons results in the exchange coupling between Sm and Co atoms. However, whether this exchange interaction of RKKY-type can produce so large strength of coupling has always been an open problem\cite{11}. In this work, we studied the electronic structure, the exchange splitting and the magnetic moment of SmCo$_{7-x}$Ti$_x$ alloy using the spin-polarized Multi-Scattering-X$\alpha$ method. The results presented here may be helpful not only to the understanding of Ti substitution effects on the electronic structure and magnetic properties of SmCo$_{7-x}$Ti$_x$ alloy, but also in presenting an insight into synthesizing Sm(Co, M)$_7$-series high temperature permanent magnetic materials.

1 Model

The crystal structure of SmCo$_{7-x}$Ti$_x$ is that of TbCu$_7$-type (space group: P6/mmm)\cite{4,9}, in which the Sm$_5$Co$_{28}$Ti$_6$ cluster possessing the symmetry of D$_{2h}$ space group is a basic unit. In the cluster, the symmetry of Sm, Co(2c) and Co(3g) sites is the same as that of the Sm$_5$Co$_{34}$ cluster from SmCo$_7$ alloy\cite{12}. However, two dumbbell-atom pairs of Co-Co and two Co(3g) atoms are substituted by Ti. The lattice parameters of SmCo$_{7-x}$Ti$_x$ alloy come from the experiment values\cite{4,9}. Due to Sm being the sixth element of lanthanum series, Sm(4f$^6$) has been treated as valence orbital. So we chose the valence electrons of Sm, Co and Ti atoms to be 4f$^6$5s$^2$5p$^6$5d$^0$6s$^2$, 3d$^7$4s$^2$ and 3d$^2$4s$^2$, respectively. The other electrons are treated as core electrons. The atomic radii of Sm, Co and Ti are taken to be 0.1385 nm, 0.0943 nm and 0.1064 nm respectively. Muffin-tin potentials in our calculation are used. The exchange parameters $\alpha$ are taken from the compilations of Schwarz\cite{13}. The partial waves are included up to $L = 3$ for the Sm, Co and Ti atoms, and up to $L = 4$ for the out-sphere regions.

2 Results and discussions

2.1 Magnetic moments

The results show that the spin magnetic moments of Sm and Co atoms are antiparallel to each other in SmCo$_{7-x}$Ti$_x$. The atomic valence, number of valence electrons and atomic magnetic moments in the alloy are shown in Table 1. One can find in the table that the net-spin magnetic moment on Sm in the alloy is $-1.75\mu_B$, wherein the contributions of 4f electrons are $-0.89\mu_B$. The spin moments of 5d electrons are parallel with that of 4f electrons, but antiparallel with that of 5p and 6s. The contributions of 6s to the magnetic moment primarily come from the spin polarization effects of conductive electrons. The 5d-orbital is the outermost layer on Sm in the SmCo$_{7-x}$Ti$_x$ alloy, and therefore it is strongly unlocalized. Thus the 5d-orbital moment is quenched almost completely. The results in this work also showed that certain 4f electrons have unlocalized characteristic to some extent, which makes those 4f electrons very near the Fermi level. Basing on Magnetism Theory and Hubbard Model and considering the localized properties of 4f electrons, we got the orbital magnetic moment on Sm in the alloy to be $3.086\mu_B$. So the atomic magnetic moment on Sm should be $1.33\mu_B$ in the alloy that is in agreement well