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MAGNETIC AND TRANSPORT PROPERTIES OF $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ IN VIEW OF KKR-CPA RESULTS

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We present results of the electronic structure study for the solid solution $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ (space group $P\bar{6}2m$). The samples were synthesized for $x = 0.0$ up to 0.15. From the electrical conductivity measurements on these materials, it was verified that resistivity increases with increasing temperature up to the Curie point T_C and changes the slope at T_C decreasing when temperature is raised above T_C . To get insight into the possible origin of such observations, we carried out the Korringa-Kohn-Rostoker-coherent potential approximation electronic structure calculations for $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ in the range of concentration $x = 0.0$ up to 1.0. It was found that alloying with Ni in Fe_2P causes vanishing of spin band splitting and non-rigid band behaving of electronic valence states near the Fermi level. The polarization factor for electrons at E_F changes in $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ with increasing x , and interestingly, it reaches maximum at $x = 0.1$, closely to the concentration ($x = 0.08$), when the largest value of T_C and a kink in temperature dependent resistivity were detected.

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1. Introduction

The T_2D hexagonal systems (space group $P\bar{6}2m$), where T represent $3d$ (Mn, Fe, Co, Ni) or $4d$ (Ru, Rh) transition metal elements, and D are metalloids (Si, P, As), exhibit complex behaviour of some measured quantities. The structural, magnetic and transport properties were investigated by various experimental techniques (neutron diffraction measurements, Mössbauer effect, specific heat, electrical resistivity, magnetization measurements) [1, 2], as well as by the

band theory methods [3–5]. In general, T_2P compounds form solid solutions with the same crystal structure. Nevertheless, when alloying with others metalloids, e.g. as in $MnFeP_{1-x}As_x$, or as in $Fe_2P_{1-x}Si_x$, the phase transition to *orthorhombic* structure is observed. The system $(Fe_{1-x}Ni_x)_2P$ is particularly attractive in that class of materials. It is observed here that the Curie temperature T_C changes with increasing x (at $x = 0.1$, T_C reaches the maximum value), while the total magnetic moment decreases monotonically [6]. This experimental observation well corresponds to the temperature dependent electrical resistivity curves [6], which show clearly a kink around T_C , the most distinct for $(Fe_{0.9}Ni_{0.1})_2P$ alloy. The present paper gives additional information on electronic structure of disordered $(Fe_{1-x}Ni_x)_2P$ samples and reveals specific features on densities of states (DOS) at the Fermi level (highly spin-polarised state), which may affect transport phenomena (resistivity, magnetoresistance).

2. Results and discussion

We performed regular band structure studies of $(Fe_{1-x}Ni_x)_2P$ (for $x = 0.0, 0.05, \dots, 1.0$) alloys using charge and spin selfconsistent Korringa–Kohn–Rostoker (KKR) method with the coherent potential approximation (CPA) [7, 8], designed to disordered systems. In fact, the Ni impurities were diluted on nonequivalent tetrahedral ($3f$) and pyramidal ($3g$) positions, thus the chemical formula $(Fe_{1-x}Ni_x)(Fe_{1-y}Ni_y)P$ better corresponds to the studied system. At present, we restrict our calculations to the case when $x = y$ (no site preference in occupancy), which is not fully supported by neutron diffraction and Mössbauer studies [9]. The experimental crystal data determined for Fe_2P system [5] were used in all computations for intermediate compositions. In Fig. 1 we see the concentration dependent total and atomic magnetic moment variations in $(Fe_{1-x}Ni_x)_2P$ system. In pure Fe_2P the local magnetic moment $2.33\mu_B$ on $Fe(3g)$ is almost three times larger than the one $0.83\mu_B$ on $Fe(3f)$ [5]. These values remain almost constant up to $x = 0.5$. For higher concentration of Ni the local moments strongly drop, nevertheless $Fe(3g)$ impurities in Ni_2P still maintain the magnetic moment $1.2\mu_B$,

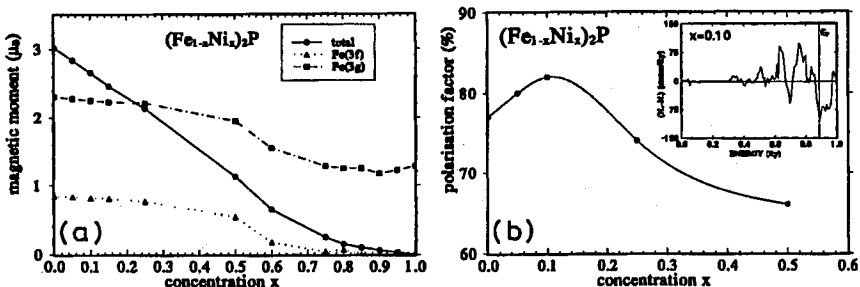


Fig. 1. (a) The total and atomic magnetic moments variations in $(Fe_{1-x}Ni_x)_2P$ system calculated from -CPA method. (b) The concentration dependent polarization factor P of electrons at E_F . In the top-right corner, the energy distribution of the total magnetic moment $\Delta N(E)$ for $(Fe_{0.9}Ni_{0.1})_2P$ is shown.

while μ_{Fe} on (3f) site indeed disappears. From the previous magnetization measurements [6], the samples with x above 0.8 exhibit zero magnetization. At this composition the iron atoms are probably diluted too much to preserve ferromagnetic (FM) ordering. The site preference in occupancy may also result into the quicker dropping of the total magnetic moment. The KKR calculations performed for ordered FeNiP (Fe at tetrahedral site, Ni at pyramidal site) and NiFeP (Ni at tetrahedral site and Fe at pyramidal site) show significantly different magnetic moments (total and atomic): 2.91, 0.86, 0.20 and 4.18, -0.12, 1.59 (in μ_{B}), respectively. In FeNiP the μ_{Ni} has parallel alignment to the μ_{Fe} , while in NiFeP compound Ni atoms possess small negative magnetic moment. From the KKR-CPA computations for the disordered $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ system, we see no magnetic moment on Ni atoms in the whole range of x concentration. In this context a polarised neutron diffraction studies will be very helpful to distinguish the atomic contributions to the total magnetic moment. Also the total energy KKR-CPA analysis of systems $(\text{Fe}_{1-x}\text{Ni}_x)\text{FeP}$, $\text{Fe}(\text{Fe}_{1-y}\text{Ni}_y)\text{P}$ and $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ is projected to observe the possible onset of site preference with Ni substitution. In Fig. 2 we present the evolution of electronic structure in $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ system. At the first sight, we observe striking differences of DOS curves at the Fermi level. For the spin-up electrons the E_{F} lies in a deep valley, while for the spin-down a large peak of DOS at E_{F} is seen.

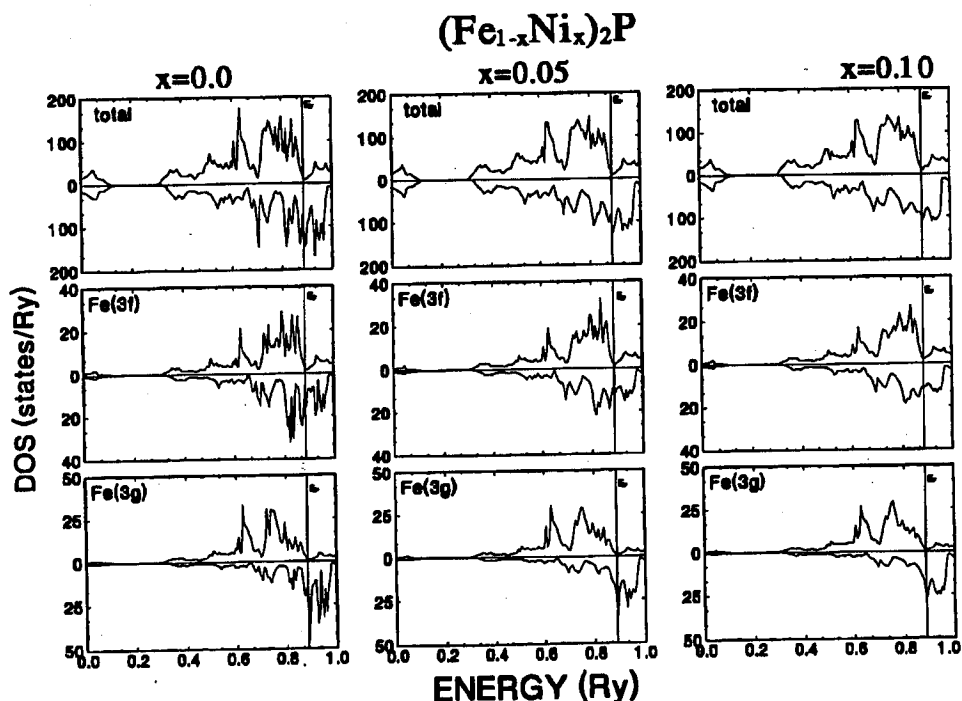


Fig. 2. The spin-projected total and component DOS for $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ ($x = 0.0, 0.05, 0.1$).

When performing the energy dependent distribution of total magnetic moment, defined as $\Delta N(E) = N_+(E) - N_-(E)$, we observe that conduction electrons near E_F possess opposite spin to the μ_{tot} , due to the large spin-down $3d$ -DOS peak seen on $\text{Fe}(3g)$. With an increase in Ni in $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$, we observe vanishing of spin band splitting and non-rigid behaving of valence bands near the Fermi level. Considering our electrical resistivity data of hexagonal systems as well as for instance $\text{Fe}_{3-x}\text{V}_x\text{Si}$ Heusler system [10], some common features can be noticed such as a maximum on resistivity curve $R(T)$ close to T_C . The DOS curves of $\text{Fe}_{3-x}\text{V}_x\text{Si}$ system is close to the half-metallic ferromagnets, which exhibit 100% polarization of electrons at E_F (a gap for one spin direction). Using the polarization factor P , defined as $P = \left| \frac{N_+(E_F) - N_-(E_F)}{N_+(E_F) + N_-(E_F)} \right| 100\%$, the polarization degree of electrons at the Fermi level can be determined. Thus, the $(\text{Fe}_{1-x}\text{Ni}_x)_2\text{P}$ can be classified as the highly spin-polarised system with the P factor above 80% (Fig. 1) in the range of $0.0 < x < 0.15$, reaching at maximum $P = 82\%$ for $(\text{Fe}_{0.9}\text{Ni}_{0.1})_2\text{P}$. This result closely relates to the anomalous behaviour of $R(T)$ curves with the maximum at T_C , which is the most pronounced for $x = 0.08$.

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