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STUDY OF CERTAIN FEATURES OF THE ELECTRONIC STRUCTURE OF THE TERNARY ALLOYS Ni<sub>3</sub>(Mn, Fe) and Ni<sub>3</sub>(Mn, Co)

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(NASA-TM-76620) STUDY OF CERTAIN FEATURES OF THE ELECTRONIC STRUCTURE OF THE TERNARY ALLOYS Ni<sub>2</sub>(Mn, Fe) AND Ni<sub>3</sub>(Mn, Co) (National Aeronautics and Space Administration) 11 p HC A02/MF A01

N82-11180

Unclass

CSSL 11F G3/26 01217

Translation of "Issledovanie nekotorykh osobennostey elektronnoy struktury troynykh splavov Ni<sub>3</sub>(Mn, Fe) and Ni<sub>3</sub>(Mn, Co)", Metallofizika, No. 37, 1971, pp. 18-22



NATIONAL AERONAUTICS AND SPACE ADMINISTRATION WASHINGTON, D.C. 20546 SEPTEMBER 1981

1. Report No. NASA TM-76620	2. Government Accession No.	3. Recipient's Catalog No.	
4. Title and Subtitle STUDY OF CERTAIN FEATURES OF THE ELECTRONIC STRUCTURE OF THE TERNARY ALLOYS Ni <sub>3</sub> (Mn, Fe) and Ni <sub>3</sub> (Mn, Co)		5. Report Date September 1981	6. Performing Organization Code
		8. Performing Organization Report No.	
7. Author(s) V. M. Zhukova and V. P. Fadin		10. Work Unit No.	
		11. Contract or Grant No. NASW-3199	
9. Performing Organization Name and Address Leo Kanner Associates Redwood City, California 94063		13. Type of Report and Period Covered	
		Translation	
12. Sponsoring Agency Name and Address National Aeronautics and Space Admini- stration, Washington, DC 20546		14. Sponsoring Agency Code	
		15. Supplementary Notes  Translation of "Issledovanie nekotorykh osobennostey elek- tronnoy struktury' troynykh splavov Ni <sub>3</sub> (Mn, Fe) and Ni <sub>3</sub> (Mn, Co)" Metallofizika, No. 37, 1971, pp. 18-22.  (A7.2-35518)	
16. Abstract Study of the changes in electronic structure related to trans- port phenomena occurring during the alloying of the alloy Ni <sub>3</sub> Mn with iron and cobalt and during the ordering of the ternary alloys thus formed. This study is performed by measuring the Hall effect, the absolute thermal emf, the in- ternal saturation induction, the Nernst-Ettingshausen constant, and the electrical resistivity. It is shown that, when the alloy Ni <sub>3</sub> Mn is alloyed with iron and cobalt and the ternary alloys thus formed become ordered, a decrease in the contri- bution of hole sections of the Fermi surface to transport phenomena occurs together with a considerable increase in the contribution of electron sections. In this case, the mobility of 3d holes decreases and the mobility of 4s electrons increases considerably.			
17. Key Words (Selected by Author(s))		18. Distribution Statement  Unclassified-Unlimited	
19. Security Classif. (of this report)  Unclassified	20. Security Classif. (of this page)  Unclassified	21. No. of Pages	22.

STUDY OF CERTAIN FEATURES OF THE ELECTRONIC STRUCTURE OF THE TERNARY ALLOYS  $Ni_3(Mn, Fe)$  and  $Ni_3(Mn, Co)$

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1. The alloy  $Ni_3Mn$  is a typical ordered alloy of transition metals. It is shown in a series of studies [1-5] that alloying of the alloy  $Ni_3Mn$  with iron and cobalt affects many of its properties differently, specifically the parameters of the electronic structure, which are associated with transport phenomena [2-4]. The nature of the indicated effect is not clear.

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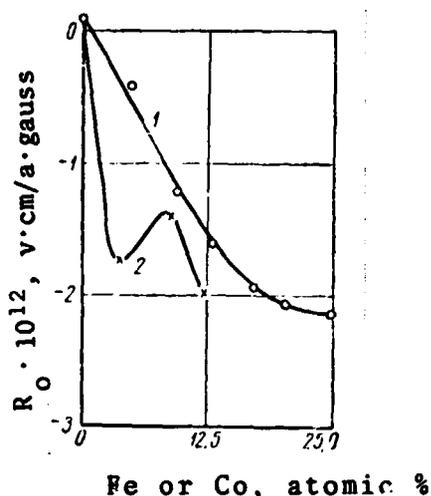


Figure 1

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Table 1

No. of Alloys	Ni	Mn	Fe	Co
1	75,0	25,0	—	—
2	74,8	20,4	4,8	—
3	75,0	16,0	9,0	—
4	74,3	12,4	13,3	—
5	74,5	9,4	16,1	—
6	74,5	6,3	19,2	—
7	75,0	—	25,0	—
8	75,0	21,0	—	4,0
9	75,0	16,0	—	9,0
10	75,0	12,5	—	12,5

One may obtain the most complete information on the electronic structure of the metals by using the anomalous skin effect method, the de Haas-Van Alfen effect method, the magnetic acoustic effect method, and others. However, the enumerated methods are applicable for materials for which large times of relaxation of the electrons of conductivity are characteristic. Therefore, they are unsuitable for the study of the electronic structure of alloys (especially alloys of transition metals). The methods of measurement of the Hall effect, the absolute thermoelectromotive force  $S$ ,

\*Numbers in the margin indicate pagination in the foreign text.

the internal saturation induction  $B_s$ , the Nernst-Ettingshausen constant  $Q_0$  and the specific resistivity  $\rho$  are very sensitive to changes in the electronic structure of the alloys [6].

In the current study, the indicated methods were used to study the change in certain parameters of the electronic structure, associated with transport phenomena, for alloying of the alloy  $Ni_3Mn$  with iron and cobalt and for ordering of the ternary alloys which form in this case.

2. The composition of the studied alloys, in atomic %, is given in table 1. The alloys were smelted in an induction furnace from initial materials of technical purity (alloys with iron), and a purity of 99.99% (alloys with cobalt). The ingots of the alloys were forged into bars after homogenization (at  $1200^\circ C$  for three days), and then rolled out into a strip 0.12 to 0.10 mm thick.

Utilized as the characteristics of state of the alloys were the magnitudes of  $S$ ,  $\rho$ , and  $Q_0$  listed above, and the normal Hall constant  $R_0$ .

The Hall and Nernst-Ettingshausen electromotive forces were measured on three-lobed samples according to the procedure in [7,8]. The procedure of measurements for  $S$  and  $\rho$  is described in [4].

The disordered state of the alloys was achieved by their heating to  $1000^\circ C$ , holding at the given temperature for two hours, and subsequent water quenching. Ordering of the alloys was carried out according to the conditions described in [3].

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3. According to the four-band model of metals and alloys [9], in the case of negligibly small conductivity of the 3d band, the relationship

$$n_s \ll n^* \ll n_d \quad (1)$$

is fulfilled, where  $n_s$  is the number of s-electrons, and  $n^*$  is the

effective number of charge carriers in the metal or alloy. Consequently, relationship (1) may serve as the criterion of the relative contribution of the holes to the transport phenomena of the metals and alloys. In the case where relationship (1) is not fulfilled for the studied metal or alloy, then holes make a substantial contribution to the transport phenomena. The effective number of charge carriers may be calculated according to the relationship [10]

$$n^* = \frac{-1}{R_0 n e} \quad (2)$$

where  $e$  is the electron charge, and  $n$  is the number of atoms per unit of volume of metal or alloy.

Presented in figure 1 are the concentration dependences of  $R_0$  for the disordered alloys of quasibinary section  $Ni_3Mn-Ni_3Fe$  (curve 1) and  $Ni_3Mn-Ni_3Co$  (curve 2). It is evident that alloying of the alloy  $Ni_3Mn$  with iron and cobalt has a substantially different effect on the nature of the change in the normal Hall constant  $R_0$ . If the concentration dependence of  $R_0$  of the alloys with iron has a monotonously diminishing nature, then, in the case of alloys with cobalt, it drops to  $C \approx 4$  atomic % Co, increases with 4 atomic % Co  $< C < 9$  atomic %, and then decreases again.

Given in table 2 are the values of  $R_0$ ,  $n^*$ ,  $n_s$  and  $Q_0$  for the studied alloys.

Table 2

No. of Alloys	Disordered				Ordered			
	$R_0 \cdot 10^{12}$ v·cm/a·Gs	$n^*$ , el/at	$n_s$ , el/at	$Q_0 \cdot 10^5$ cm <sup>2</sup> /s·deg	$R_0 \cdot 10^{12}$ v·cm/a·Gs	$n^*$ , el/at	$n_s$ , el/at	$Q_0 \cdot 10^5$ cm <sup>2</sup> /s·deg
1	- 0,09	- 7,79	0,50	6,1	- 0,95	0,74	0,7	0,9
2	- 0,41	1,74	0,52	4,6	- 1,89	0,37	0,7	2,1
3	- 1,21	0,58	0,57	2,9	- 1,87	0,38	0,7	1,0
4	- 1,65	0,43	0,58	2,0	- 1,22	0,42	0,7	12,8
5	- 1,88	0,37	0,60	4,2	- 1,29	0,55	0,7	11,0
6	- 2,03	0,35	0,61	12,0	- 1,77	0,40	0,7	21,3
7	- 2,13	0,33	0,65	45,0	- 1,98	0,33	0,7	45,3
8	- 1,76	0,40	0,52	2,8	- 1,87	0,38	-	-
9	- 1,36	0,52	0,54	- 2,7	- 1,99	0,32	-	-
10	- 1,99	0,36	0,56	1,1	- 2,45	0,30	-	-

According to the data in [11].

The very small positive value of  $R_0$  (see table 2 and figure 1) for the disordered alloy  $Ni_3Mn$  indicates the slightly differing contributions of the hole and electron sections of the Fermi surface (PF) in it. In this case, it is necessary to note that the sign of  $R_0$ , in the general case, depends on the tensor of the inverse effective mass  $1/m^*$ . If the Fermi surface differs considerably from a sphere, then the components of the tensor may have different signs in different (or even in the same) sections of the Fermi surface. Therefore, individual sections of the electron Fermi surface may give a positive contribution to  $R_0$ , while individual sections of the hole Fermi surface may give a negative contribution. However, a large portion of the electron Fermi surface gives a negative contribution, and the hole Fermi surface gives a positive contribution, to  $R_0$ . Consequently, hole (3d-holes) sections of the Fermi surface make a substantial contribution to the transport phenomena of the disordered alloy  $Ni_3Mn$ .

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The replacement of a relatively small amount ( $C \leq 4.8$  atomic %) of manganese in the alloy  $Ni_3Mn$  with iron disrupts the approximate equality of the contributions of the electron and hole sections of the Fermi surface to  $R_0$ . Therefore, in spite of the slight changes in the structure of the 3d-band in this case [2-4], there occurs a considerable change in  $R_0$  (see figure 1 and table 2). Similar effects were observed in a number of other alloys (during their alloying), and in metals as well (with a change in temperature) [9, 12, 13].

It is evident from analysis of the data in table 2 that, for the ternary alloys  $Ni_3(Mn, Fe)$  with a relatively small iron concentration, condition (1) is not fulfilled. Consequently, in the indicated alloys (in spite of the negative values of  $R_0$ ), the hole sections of the Fermi surface make a substantial contribution to the transport phenomena. With a subsequent increase in the iron concentration ( $C > 4.8$  atomic %) in the alloys  $Ni_3(Mn, Fe)$ , the contribution of the hole sections of the Fermi surface to  $R_0$  decreases (and the contribution of the electron sections increases

accordingly), and with C=9 atomic %, Fe becomes negligibly small. As is evident from table 2, for the latter alloy,  $n^* \approx n_s$ . Consequently, only the s-electrons are charge carriers in the given alloy, and, according to [9], the relaxation times of the s-electrons, in both directions of spin, should be roughly equal ( $\tau_{s\uparrow} \approx \tau_{s\downarrow}$ ). The following relationships are obtained in [14]:

$$\begin{aligned} 1/\tau_{s\uparrow}(E_F) &\sim N_{d\uparrow}(E_F) + \beta, \\ 1/\tau_{s\downarrow}(E_F) &\sim N_{d\downarrow}(E_F) + \beta, \end{aligned} \quad (3)$$

where  $N_{d\uparrow}(E_F)$  and  $N_{d\downarrow}(E_F)$  are the densities of electron states in the  $d\uparrow$ - and  $d\downarrow$ -bands, respectively,  $E_F$  is the Fermi energy, and  $\beta$  is the contribution to s-electron scattering because of the s-s-transitions, which is usually equal for both directions of spin.

It follows from (3) that, for the alloy Ni + 16 atomic % Mn + 9 atomic % Fe,  $N_{d\uparrow}(E_F) \approx N_{d\downarrow}(E_F)$ , which agrees with the nature of the concentration dependence of the internal saturation induction of  $Ni_3(Mn, Fe)$  alloys [3]. Evidently, the Fermi level of the given alloy in the  $3d\downarrow$ -band is located to the right of the highest maximum on the curve  $N_d=f(E)$  [14, 2-4].

A further decrease in  $R_0$ , with an increase in the iron concentration in the  $Ni_3(Mn, Fe)$  alloys, is evidently brought about basically by a decrease in  $N_{d\downarrow}(E_F)$ , since  $N_{d\uparrow}(E_F)$  changes weakly in this case [2-4].

The value  $n^* \approx n_s/2$  (see table 2) for the alloy  $Ni_3Fe$  indicates that the  $3d\downarrow$ -band is filled, and  $N_{d\downarrow}(E_F)=0$ . Therefore, the  $4s\downarrow$ -electrons of the given alloy may be scattered only into the  $4s$ -band with a low density of state, as a result of which they have a high mobility and give a basic contribution to  $R_0$ , by lowering it.

The monotonous and smooth nature of the concentration dependence of the  $R_0$  of the  $Ni_3Mn-Ni_3Fe$  alloys of quasibinary cross section

indicates the presence of a closed Fermi surface in the indicated alloys. Actually, if the Fermi surface in the alloy  $Ni_3Mn$  were open, then, with its alloying with iron, the Fermi surface contact with the boundary of the zone (and therefore the contribution of the holes to  $R_0$ ) should increase. Therefore,  $R_0 > 0$  should also increase. The experimental data show a sharp decrease in  $R_0$  and the contribution of the holes to  $R_0$ . The conclusion on a closed Fermi surface in the given alloys agrees with the results in [4], obtained on the basis of analysis of the experimental values of  $S$  and  $\rho$ , and for the alloy  $Ni_3Fe$ —with the results in [16]. The comparison of the results, obtained by two (and for the alloy  $Ni_3Fe$ —by three) independent experimental methods, indicates their sufficient reliability.

The sharp reduction in  $R_0$  with alloying of the alloy  $Ni_3Mn$  with small cobalt additives (curve 2 in figure 1) is evidently brought about by the sharp increase in the contribution of the electron sections of the Fermi surface to the transport phenomena, which is associated with the introduction of two additional 3d-electrons by each cobalt atom (instead of the one introduced by an iron atom) into the 3d-band of the  $Ni_3Mn$  alloy. The nature of the subsequent nonmonotonous course of the concentration dependence of  $R_0$  (just as that of a number of other characteristics [3, 5]) still remains somewhat unclear.

The changes in the contributions of the electron and hole Fermi surfaces to the transport phenomena may be brought about by a change in both the number of charge carriers, and their

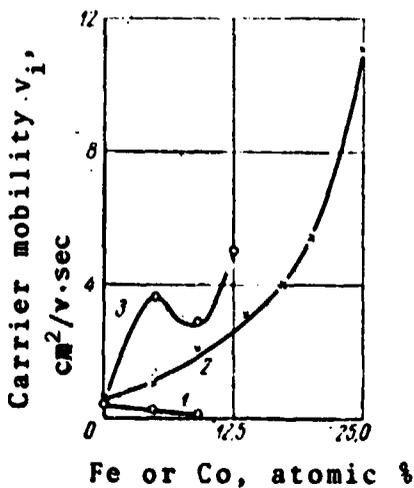


Fig. 2

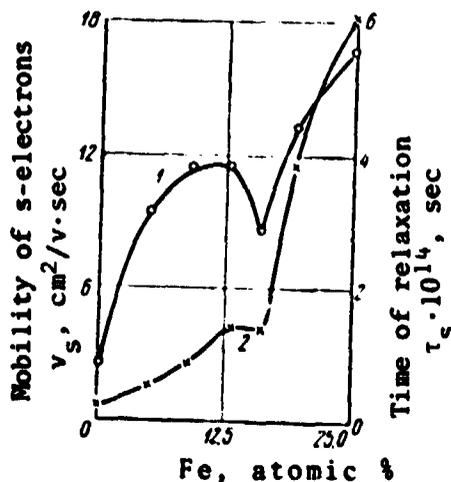


Fig. 3

mobilities. In this case, the Fermi levels in the d- and s-bands should also change. In order to determine the indicated magnitudes, it is necessary to know the values of  $S$ ,  $R_0$ ,  $Q_0$  and the specific electrical conductivity  $\sigma$  for the studied alloys. The values of  $S$  are taken from [4], the values of  $\sigma$  are calculated according to the values of  $\rho$  [4], and  $R_0$  and  $Q_0$  are measured in the given study, and given in table 2. By utilizing the experimentally measured values of the indicated magnitudes, one can use the relationships in [17-20] to determine the values of the mobilities of the 4s-electrons and the 3d-holes in the studied alloys. The results of the calculations are given in figure 2. It is evident that a decrease in the contribution of the hole sections of the Fermi surface, and an increase in the contribution of the electron sections of the Fermi surface, to the transport phenomena during alloying of the alloy  $Ni_3Mn$  with iron is brought about basically by a decrease in the mobility of the 3d-holes (curve 1), and by an intensive increase in the mobility of the 4s-electrons (curve 2). The still more intensive mobility of the s-electrons  $v_s$  increases with alloying of the  $Ni_3Mn$  alloy with cobalt (curve 3), although the concentration dependence of  $v_s$  is not monotonous here. The mobility of the d-holes in the latter case also falls considerably more intensively than in alloys with iron.

Given in figure 3 are the concentration dependences of the mobility  $v_s$  (curve 1) and the time of relaxation  $\tau_s$  (curve 2) of the s-electrons of the  $Ni_3(Mn, Fe)$  ordered alloys of quasibinary cross-section. It is evident from comparison of the curves of  $v_s$  (see figures 2 and 3) that, with ordering of the given alloys, there occurs a considerable increase in the mobility of the s-electrons. It is evident from the data in table 2 that, even with  $C \approx 4.8$  atomic % Fe, the value of  $n^*$  approximately satisfies condition (1). This indicates the negligibly small contribution of the hole sections of the Fermi surface to the transport phenomena of the given alloy.

The trend of the curves  $v_s = f(C)$  and  $\tau_s = f(C)$  (see figure 3) agrees satisfactorily with the trend of the curve of the density

of states  $N_d=f(E)$  for the given alloys [15, 5, 4]. With alloying of the alloy  $Ni_3Mn$  with iron, the Fermi level displaces towards the top of the  $3d$ -band [5, 4], and, in this case, up to  $C=9$  atomic % Fe, there occurs a decrease in both  $N_{d\uparrow}$  and  $N_{d\downarrow}$ . Therefore, the scattering of  $s$ -electrons into the  $d$ -band decreases, while  $v_s$  and  $\tau_s$  increase accordingly. With  $C>9$  atomic % Fe, the Fermi level in the  $3d$ -band passes through a deep minimum of the curve  $N_d=f(E)$  [15, 5, 4]; therefore,  $N_{d\uparrow}$  begins to increase, while  $N_{d\downarrow}$  continues to decrease, which leads to a considerable decrease in  $v_s$ , and to a slight (very small) decrease in  $\tau_s$  (in this case, a nearly horizontal area is observed on curve 2 in figure 3). As the Fermi surface approaches the top of the  $3d$ -band,  $N_d$  rapidly decreases to zero; therefore, the scattering of  $s$ -electrons into the  $3d$ -band decreases rapidly (also to zero), and  $v_s$  and  $\tau_s$  increase, reaching maximum values in the alloy  $Ni_3Fe$ . /22

Thus, with alloying of the alloy  $Ni_3Mn$  with iron and cobalt, and with ordering of the product ternary alloys in this case, there occurs a decrease in the contribution of hole sections, and a considerable increase in the contribution of electron sections, of the Fermi surface to the transport phenomena. In this case, the mobility of the  $3d$ -holes decreases, and the mobility of the  $4s$ -electrons increases considerably. Clearly manifested on the concentration dependences of  $v_s$  and  $\tau_s$  of the ordered alloys  $Ni_3(Mn, Fe)$  is disruption of the monotonous nature, associated with the passage of the Fermi level through the point of the deep energetic minimum of the curve of density of states  $N_d=f(E)$ , obtained theoretically in [15]. The given results may serve as indirect experimental corroboration of the correctness of the calculations carried out in [15].

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