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A72-35570

NASA TECHNICAL MEMORANDUM NASA TM-76620

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

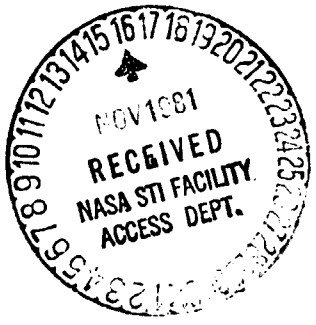
V. M. Zhukova and V. P. Fadin

(NASA-TM-76620) STUDY OF CERTAIN FEATURES OF THE ELECTRONIC STRUCTURE OF THE TERNARY ALLOYS Ni2(Mn, Fe) AND Ni3(Mn, Co) (National Aeronautics and Space Administration) 11 p HC A02/MF A01 CSCL 11F G3/26

N82-11180

Unclas 01217

Translation of "Issledovanie nekotorykh osobennostey elektronnoy struktury troynykh splavov Ni_3(Mn, Fe) and Ni_3(Mn, Co)", Metallofizika, No. 37, 1971, pp. 18-22



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

STANDARD TITLE PAGE

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_3(Mn, Fe) and Ni_3(Mn, Co)		5. Report Date September 1981 6. Performing Organization Code
7. Author(s) V. M. Zhukova and V. P. Fadin		8. Performing Organization Report No. 10. Work Unit No.
9. Performing Organization Name and Address Leo Kanner Associates Redwood City, California 94063		11. Contract or Grant No. NASw-3199 13. Type of Report and Period Covered Translation
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration, Washington, DC 20546		14. Sponsoring Agency Code

15. Supplementary Notes

Translation of "Issledovanie nekotorykh osobennostey elektronnoy struktury troynykh splavov Ni_3(Mn, Fe) and Ni_3(Mn, Co)" Metallofizika, No. 37, 1971, pp. 18-22.

(A72-35518)

16. Abstract

Study of the changes in electronic structure related to transport phenomena occurring during the alloying of the alloy Ni_3Mn 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 internal saturation induction, the Nernst-Ettingshausen constant, and the electrical resistivity. It is shown that, when the alloy Ni_3Mn is alloyed with iron and cobalt and the ternary alloys thus formed become ordered, a decrease in the contribution 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)	20. Security Classif. (of this page)	21. No. of Pages	22.
Unclassified	Unclassified		

NASA-HQ

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. /18*

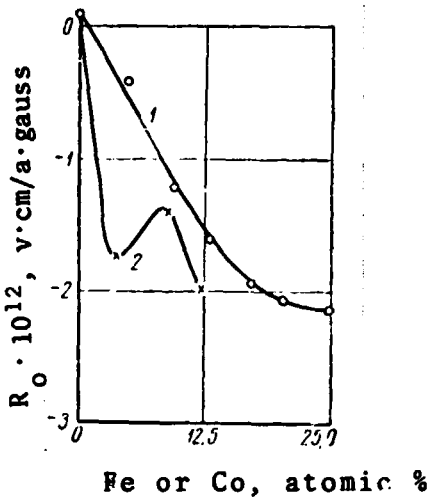

Figure 1

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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 Gaas-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 ρ 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° 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, ρ, 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 ρ is described in [4].

The disordered state of the alloys was achieved by their heating to 1000° 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]. /19

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

$$n_s \leqslant n^* \leqslant n_s \qquad (1)$$

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]

$$n^* = \frac{-1}{R_0 ne}, \qquad (2)$$

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≈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 ω_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	$Q_0 \cdot 10^5$ cm²/s·deg	$R_0 \cdot 10^{12}$ v·cm/a·Gs	n^* el/at	n_s, el/at	$Q_0 \cdot 10^5$ cm²/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	−1,52	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, /20
hole (3d-holes) sections of the Fermi surface make a substantial contribution to the transport phenomena of the disordered alloy Ni_3Mn.

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]:

$$1/\tau_{s\uparrow}(E_F) \sim N_{d\uparrow}(E_F) + \beta,$$
$$1/\tau_{s\downarrow}(E_F) \sim N_{d\downarrow}(E_F) + \beta. \qquad (3)$$

where $N_{d\uparrow}(E_F)$ and $N_{d\downarrow}(E_F)$ are the densities of electron states in the d↑- and d↓-bands, respectively, E_F is the Fermi energy, and β 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↓-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↓-band is filled, and $N_{d\downarrow}(E_F) = 0$. Therefore, the 4s↓-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 ρ, 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. /21

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

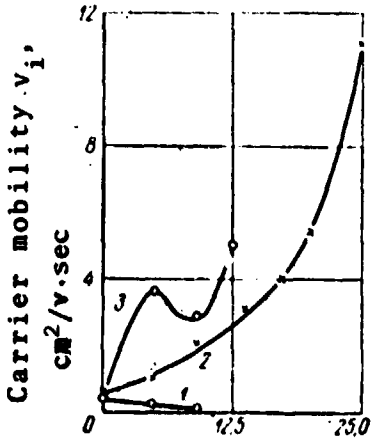

Fig. 2

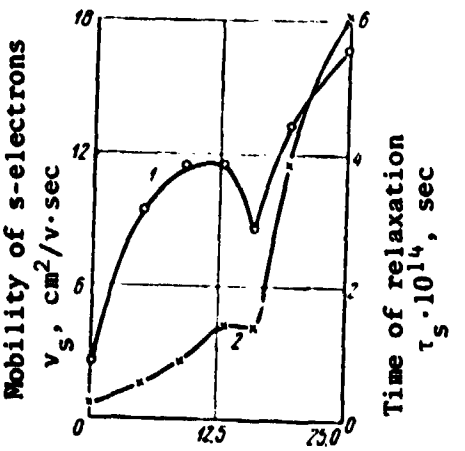

Fig. 3

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 σ for the studied alloys. The values of S are taken from [4], the values of σ are calculated according to the values of ρ [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 υ_s increases with alloying of the Ni_3Mn alloy with cobalt (curve 3), although the concentration dependence of υ_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 υ_s (curve 1) and the time of relaxation τ_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 υ_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≈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 $\upsilon_s = f(C)$ and $\tau_s = (C)$ (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 /22
scattering of s-electrons into the d-band decreases, while υ_s and τ_s increase accordingly. With C>9 atomic % Fe, the Fermi level in the $3d\downarrow$-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 υ_s, and to a slight (very small) decrease in τ_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 $3d_\downarrow$-band, $Nd_\downarrow$ rapidly decreases to zero; therefore, the scattering of s-electrons into the $3d_\downarrow$-band decreases rapidly (also to zero), and υ_s and τ_s increase, reaching maximum values in the alloy Ni_3Fe.

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 υ_s and τ_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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