

Moment-Induced Magnetic Scattering and Magnetovolume Effect in $\text{Fe}_{65}(\text{Ni}_{1-x}\text{Mn}_x)_{35}$ Alloys

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(Received July 22, 1968)

The temperature dependences of electrical resistivity and thermal expansion were measured for face-centered cubic $\text{Fe}_{65}(\text{Ni}_{1-x}\text{Mn}_x)_{35}$ ternary alloys. The electrical resistivity of ferromagnetic alloys ($x < 0.3$) decreases with increasing magnetic ordering. In contrast to this, the resistivity of antiferromagnetic alloys ($x > 0.3$) increases below the Néel temperature and shows a resistance minimum. These behaviors are explained in terms of the magnetic scattering by induced moments below the magnetic ordering temperature. The expansion of volume due to the magnetic ordering was observed in both ferro- and antiferromagnetic alloys. To explain the volume expansion by the magnetic ordering, a new mechanism of magnetovolume effect based on the change of cohesive energy due to the spin polarization in $3d$ band is proposed.

§ 1. Introduction

Several attempts have been made to explain the origin of the Invar effect, namely the low thermal expansion, the abrupt change of magnetization as a function of electron concentration, the large pressure effect on both magnetization and Curie temperature, the large volume magnetostriction and so on. Kondorsky and Sedov¹⁾ proposed an idea that there is a latent antiferromagnetism in Invar alloys. Weiss²⁾ showed that many experimental results can quantitatively be explained on the basis of the assumption that there are two electronic states of iron in face-centered cubic lattice. On the other hand, Katsuki³⁾ tried a band-theoretical explanation on the origin of the Invar effect.

Since the Invar effect is found in face-centered cubic iron alloys whose iron concentration is sufficiently high that they are very near the γ - α phase boundary in phase diagrams, it is worthwhile to study the general features of the magnetic properties for various iron rich face-centered cubic iron alloys to solve the Invar problem. The magnetic properties of ferromagnetic iron alloys with face-centered cubic structure such as FeNi and FePt alloys are quite different from those of antiferromagnetic ones such as FeMn alloys. For instance, the internal field at iron nuclei in FeNi alloys is about 300kOe^{4,5)} and those in FeMn alloys^{6,7)} and γ -iron precipitated from copper⁸⁾ are about 30kOe. Moreover, the paramagnetic susceptibility of FeNi alloys obeys the Curie-Weiss law and that of FeMn alloys is nearly temperature independent.⁹⁾

In order to clarify the origin of the Invar effect in connection with the difference of magnetic properties between ferromagnetic and antiferromagnetic face-centered cubic iron alloys, one of the present authors studied the magnetic properties of $\text{Fe}_{65}(\text{Ni}_{1-x}\text{Mn}_x)_{35}$ ternary alloys with the face-centered cubic structure¹⁰⁾ and found that these alloys are ferromagnetic in the range of $x < 0.3$ and are antiferromagnetic in the range of $x > 0.3$. In order to explain the magnetic properties of these alloys he proposed a model as to the magnetic states of FeNiMn alloys by applying the theory presented by Bailyn¹¹⁾ for the magnetic states of transition metals.

In this paper, the results of electrical resistivity and thermal expansion measurements of $\text{Fe}_{65}(\text{Ni}_{1-x}\text{Mn}_x)_{35}$ alloys are reported. The temperature dependence of electrical resistivity is well understood in terms of the magnetic scattering by induced magnetic moments below the magnetic ordering temperature.¹⁰⁾ On the other hand, the behavior of thermal expansion of these alloys, especially that of antiferromagnetic alloys, can be explained neither by the usual mechanism based on the volume dependence of exchange interaction nor by the Weiss theory.²⁾ In order to explain the magnetovolume effect observed in antiferromagnetic alloys and also in the Invar alloys, the present paper describes a new mechanism of magnetovolume effect based on the idea that the change of spin polarization in the $3d$ band induces the change of cohesive energy which reflects to a variation of the atomic distance.

§ 2. Experimental Procedures

Specimens used for electrical resistivity measurements were wires, 0.5 mm in diameter and about 50 mm in length, drawn from the same ingots used for magnetic measurements.¹⁰⁾ Specimens for thermal expansion measurements were blocks, about $5 \times 5 \times 20 \text{ mm}^3$, cut from the same ingots. Every sample was sealed into evacuated silica tube and was annealed at 1050°C for two days to homogenize the concentration of alloys and then quenched into water to get the disordered state. The compositions of the alloys are given in the Table I of the previous paper.¹⁰⁾ Electrical resistivity was measured from liquid helium temperature up to 700 K by conventional four-terminal method. Thermal expansion was measured from liquid nitrogen temperature up to 600 K using a dilatometer by which the change of length in specimens was detected by means of a differential transformer.

§ 3. Results and Discussions

3.1. Electrical resistivity

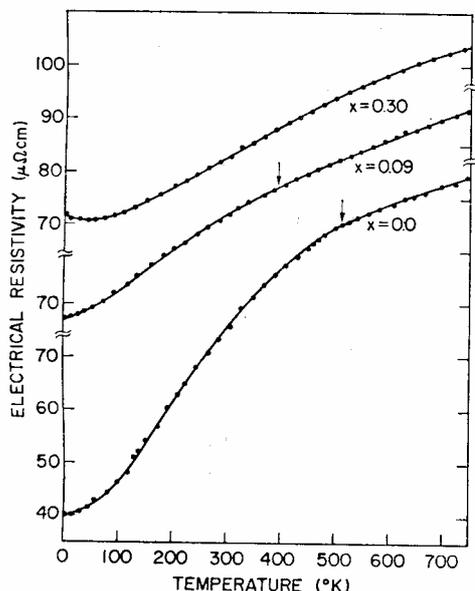


Fig. 1. The temperature dependence of electrical resistivity of ferromagnetic FeNiMn alloys. The arrow indicates the Curie temperature determined by magnetic measurements.

Figures 1 and 2 show the temperature dependence of electrical resistivity of ferromagnetic alloys ($x < 0.3$) and of antiferromagnetic alloys ($x > 0.3$), respectively. Main features of the results

are as follows: 1) The resistivity curve of ferromagnetic alloys bends downwards below the Curie temperature with decreasing temperature. This result indicates that the resistivity decreases by ferromagnetic ordering. However, the resistivity curve does not bend so sharp as that of typical

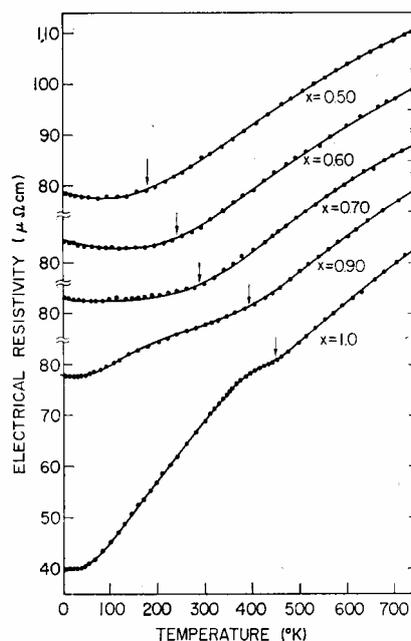


Fig. 2. The temperature dependence of electrical resistivity of antiferromagnetic FeNiMn alloys. The arrow indicates the Néel temperature determined by magnetic measurements.

ferromagnetic metals such as nickel. 2) In contrast, the resistivity curves of antiferromagnetic alloys bend upwards below the Néel temperature with decreasing temperature. This result indicates that the resistivity increases by antiferromagnetic ordering. 3) Some of the antiferromagnetic alloys exhibit the resistance minimum at fairly high temperatures of about 100 K. The first and second characteristics are usually found in ferromagnetic and antiferromagnetic alloys, respectively. However, the third characteristic is unusual. The "resistance minimum" is frequently observed in magnetic dilute alloys and is now well known as resulting from the Kondo effect.¹²⁾ However, the resistance minimum observed in the present alloys is not considered as the Kondo effect, because it is not observed in the paramagnetic state but in the antiferromagnetic one and moreover is not observed in magnetic dilute alloys but in iron rich alloys.

Now this phenomenon can be understood by the model previously proposed by one of the authors.¹⁰⁾ Bailyn¹¹⁾ analyzed the behavior of local moments of transition metals associated with the Wannier functions on the atom sites in the presence of exchange interaction. The results of his calculation are schematically shown in Fig. 3, in which the abscissa is proportional to the mo-

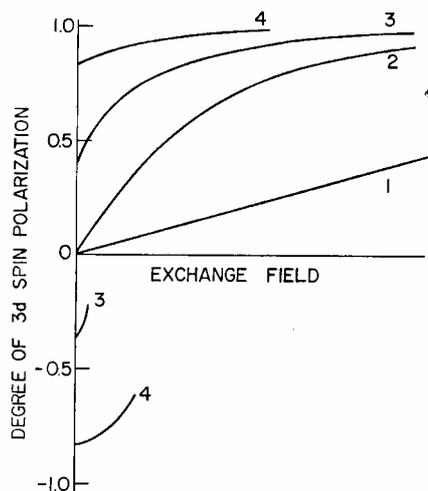


Fig. 3. Schematic representation of the result of Bailyn's theory. The ordinate is the degree of spin polarization of the Wannier function at a given atomic site. The abscissa is proportional to the effective exchange field at the atom site. Curves 1 and 2 correspond to the induced moment state. Curves 3 and 4 correspond to the permanent moment state. We believe that the local moment of iron atoms in the Invar alloy corresponds to the curve 3 and that of Ni, Co and b.c.c. Fe corresponds to the curve 4 and that of Cr and γ -FeMn to 1 or 2.

lecular field acting on local moments and the ordinate represents the degree of spin polarization of local moments. The figure shows how the local moment is induced by an exchange field determined mainly by the correlation energy. From this figure we can see the following characteristics. 1) There are two types of local moments. One is the moment having a net moment only under the presence of effective field. 2) The other is in the state where the spins of 3d electrons are spontaneously polarized or have net moments with both parallel and antiparallel directions to the effective field in paramagnetic state. We call the former "the induced moment" and the magnetic moment of chromium is probably an induced moment; we call the latter "the permanent moment" which is similar to Ander-

son's localized moment. The magnetic state indicated by the curve 3 in Fig. 3 is a permanent moment state according to our definition. However, a considerable amount of excess moment is induced by the effective field. This means that the local moment in this state increases markedly below the magnetic ordering temperature.

On the basis of the above-mentioned idea, we made three assumptions on the magnetic state of FeNiMn alloys as follows: 1) At manganese sites the local moment is an induced moment. 2) At nickel sites it is a permanent moment. 3) At iron sites the local moment is a permanent moment for ferromagnetic alloys and is an induced moment for antiferromagnetic alloys. The Invar alloys are ferromagnetic alloys as a whole but their alloy concentrations are very close to those of antiferromagnetic alloys and in actual Invar alloys the antiferromagnetic regions coexist with ferromagnetic ones.^{5,18)} Therefore, it is expected from the above-mentioned assumptions that the magnetic state of iron atoms in the Invar alloy is the state indicated by the curve 3 which means that the magnetic moment of the present Invar alloys increases below the Curie temperature. The result of neutron scattering experiment on the Invar alloy by Collins¹⁴⁾ can be regarded as an evidence of this model. On the other hand, there is no direct evidence indicating the absence of permanent moment in FeMn alloy which is expected to be in the magnetic state shown by the curve 1 or 2 in Fig. 3. It should be noted, however, that the temperature independent paramagnetic susceptibility above the Néel temperature can not be understood by a simple localized model or a permanent moment. Third assumption is supported from the fact that the internal field acting on iron nuclei changes abruptly due to the ferro-antiferromagnetic transition by a change of the composition of alloys.¹⁵⁾ We showed that this abrupt change of internal field can not be understood unless a change of electronic configuration of iron atom is assumed.

We shall show here that the unusual temperature dependence of electrical resistivity of FeNiMn alloys can well be interpreted in terms of the above-mentioned model. The main contributions to electrical resistivity of the present magnetic alloys are schematically shown in Fig. 4. The curve A represents the magnetic disorder-

dered scattering of usual magnetic metals and alloys. The residual resistivity and the phonon contribution are shown by the curve B. Therefore, the total resistivity of usual magnetic alloys can be represented by the curve C and we can not expect the appearance of any resistance minimum. In the present case, however, we must consider the effect of induced moment and of the random distribution of magnetic atoms with different

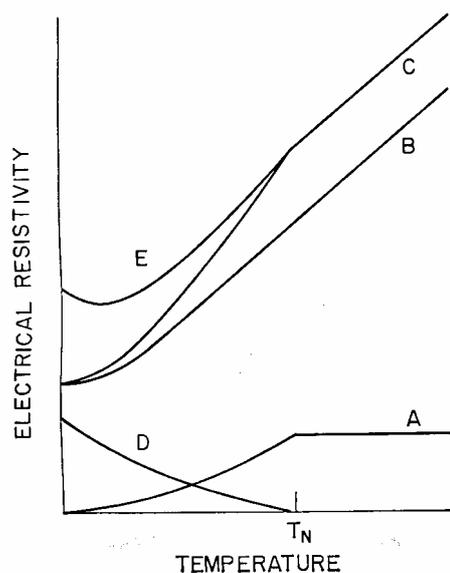


Fig. 4. Schematic resistivity curve of magnetic alloys having induced moments. Curve A indicates the magnetic disordered scattering due to the permanent moment. The residual resistivity and the phonon contribution are shown by the curve B. Curve C means the total resistivity of usual magnetic alloys. Curve D represents the magnetic resistivity due to the induced moment and random distribution of magnetic moments. The total resistivity can be shown by the curve E.

atomic moments. Above the magnetic ordering temperature, the resistivity due to magnetic scattering can not be observed in a magnetic alloy with induced moments. Below the magnetic ordering temperature, on the other hand, local moments are induced and then the magnetic scattering takes place. In the present disordered alloys this magnetic scattering does not disappear at low temperatures, because the randomness of magnetic moments still remains even at 0 K. This effect is schematically shown by the curve D. According to our assumptions on the magnetic states of the present alloys, the contribution to

resistivity represented by the curve A comes from only nickel atoms in the antiferromagnetic alloys. Therefore, the contribution of the curve A may be small. On the other hand, the curve D involves both iron and manganese atoms whose concentrations are fairly high as compared with nickel. It turns out that the contribution of the curve D is larger than that of the curve A and a resistance

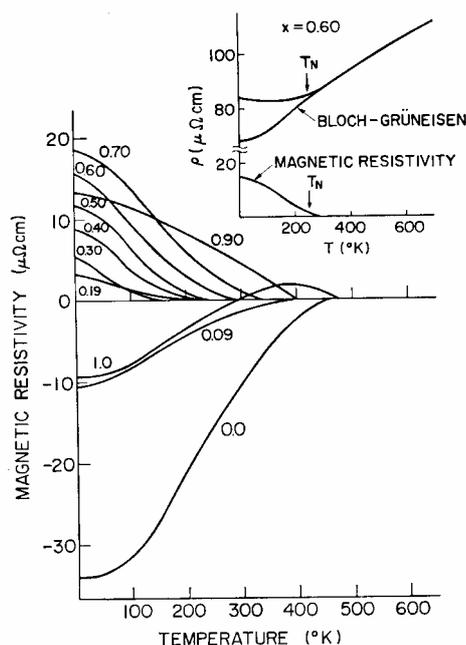


Fig. 5. The temperature dependence of magnetic resistivity of FeNiMn alloys. The magnetic resistivity was obtained by subtracting the phonon contribution and residual resistivity using the Bloch-Grüneisen formula. This procedure is shown for $x=0.60$ in the upper part of the figure.

minimum can be observed as shown by the curve E.

The magnetic contribution to electrical resistivity was evaluated from the observed resistivity as follows. The phonon part of resistivity obeys the Bloch-Grüneisen formula in which the Debye temperature was estimated by interpolating the Debye temperature of FeMn and FeNi¹⁶⁾ and the other parameter was estimated by adjusting it to get the best-fit to the respective slope of the linear part of the observed resistivity just above the magnetic ordering temperature. By subtracting the phonon part and the residual resistivity thus obtained from the observed resistivity, we can get the temperature dependence of magnetic part or

resistivity below the magnetic ordering temperature. Figure 5 shows the temperature dependence of magnetic resistivity for each sample and an example of this procedure for the alloy with $x=0.60$. As seen from the figure, the magnetic contribution to electrical resistivity in antiferromagnetic alloys increases with increasing manganese concentration. However, it begins to decrease from $x=0.90$ and changes its sign for FeMn alloy. If the magnetic scattering mechanism in transition metals and alloys proposed by Weiss and Marotta¹⁷⁾ is valid, this result suggests that the local moment of the iron atom is nearly the same as that of the manganese atom and therefore the above mentioned effect on magnetic resistivity shown by the curve D in Fig. 4 becomes very small. Thus, we believe that the magnetic diffuse scattering is not expected in FeMn alloy.

The magnetic residual resistivity of antiferromagnetic alloy with $x=0.60$ is about $15 \mu\Omega\text{cm}$. According to Weiss and Marotta,¹⁷⁾ the magnetic residual resistivity, $\rho_{0\text{mag}}$, can be expressed as

$$\rho_{0\text{mag}} = Cx_Ax_B(S_A - S_B)^2,$$

where C is the constant, x_A and x_B the mole fraction of constituent atoms and S_A and S_B the spin on the A and B atom, respectively. Assuming that $S_A=S_{\text{Fe}}=S_{\text{Mn}}$, $S_B=S_{\text{Ni}}$ and $S_A-S_B=1$, we obtain $\rho_{0\text{mag}}=3.5 \mu\Omega\text{cm}$ for the alloys with $x=0.60$ where $x_A=x_{\text{Fe}}+x_{\text{Mn}}=0.86$ and $x_B=x_{\text{Ni}}=0.14$. This value is smaller than the experimental one. Considering roughness of estimation, however, these values seem to be in good agreement. Thus, the unusual electrical resistivity of antiferromagnetic alloys can well be interpreted in terms of our model.

As shown in Fig. 1, the general feature of magnetic resistivity of ferromagnetic alloys is similar to those of typical ferromagnetic metals, although a discontinuous change of the slope at the Curie temperature is not found. This behavior can be understood as being originated from the local fluctuation of the concentration. However, it is also explained from our model as shown in Fig. 6. In the case of the permanent moment, the magnetic resistivity changes with temperature as shown by the curve A. In the Invar alloys, however, the considerable amount of magnetic moment is induced below the Curie temperature and

this increase of the magnetic moment is reflected in the electrical resistivity as shown by the curve B or B'. The residual resistivity and the phonon contribution are shown by the curve C. Then, the total resistivity can be represented by the curve D or D'. It should be noted that an upward deviation of electrical resistivity below the Curie temperature can be expected under a suitable condition as shown by the curve D' in the figure. Actually, this upward deviation was found in FeCoCr alloys¹⁸⁾ which have the Invar character.

The magnetic resistivity of ferromagnetic alloys decreases with increasing manganese concentra-

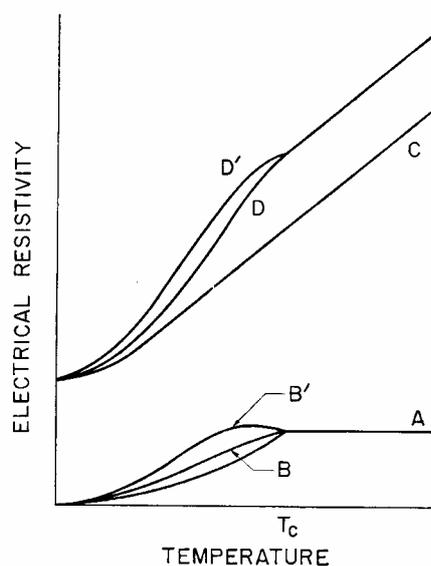


Fig. 6. Schematic resistivity curve for ferromagnetic Invar alloys. Curve A indicates the magnetic scattering due to the permanent moment. The contribution of the induced moment is shown by the curve B or B'. The residual resistivity and phonon contribution are shown by curve C. The total resistivity curves D and D' correspond to B and B', respectively.

tion and becomes positive for $x=0.19$, though the alloy is still ferromagnetic. This result may arise from the fact that the amount of induced moment below the Curie temperature increases with increasing manganese concentration and the above-mentioned effect shown by the curve D in Fig. 4 becomes significant. This result can also be explained by coexistence of antiferromagnetic regions with ferromagnetic ones.^{5,18)}

3.2. Thermal expansion

Figures 7 and 8 show the results of thermal expansion measurements of ferromagnetic alloys

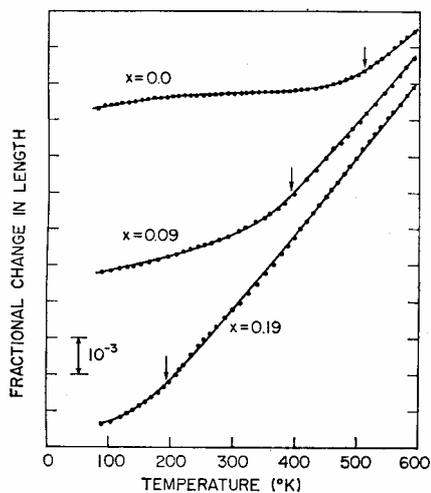


Fig. 7. The temperature dependence of thermal expansion of ferromagnetic FeNiMn alloys. The arrow indicates the Curie temperature determined by magnetic measurements.

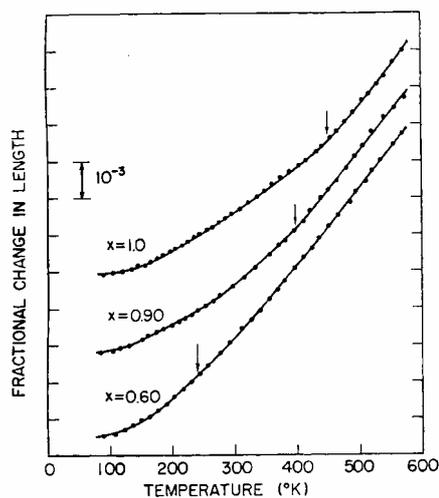


Fig. 8. The temperature dependence of thermal expansion of antiferromagnetic FeNiMn alloys. The arrow indicates the Néel temperature determined by magnetic measurements.

and antiferromagnetic ones, respectively. The main characteristics are as follows: 1) The Invar effect, in other words, the volume expansion due to the magnetic ordering was found in all of the ferromagnetic alloys. 2) Thermal expansion-curves of antiferromagnetic alloys also show the volume expansion below the Néel temperature. This volume expansion is much smaller than that of ferromagnetic alloys. 3) The volume expansion decreases with increasing x for ferromagnetic alloys and with decreasing x for antiferromagnetic alloys. It increases with increasing the

magnetic ordering temperature for both types of alloys. It was confirmed that the extra volume expansion of ferromagnetic alloys is proportional to the square of spontaneous magnetization. This fact shows that the extra volume expansion originates from the magnetic ordering. The details of this work will be published elsewhere.

On the basis of the molecular field theory of ferromagnetism, the magnetovolume effect can be interpreted in terms of the volume dependence of the exchange integral. The volume change due to the ferromagnetic ordering, $\omega(M)$, is given by

$$\omega(M) = CM^2 \alpha \frac{dJ}{d\omega},$$

where C is the compressibility, M the magnetization, α a positive constant and J the exchange integral. Similarly, the antiferromagnetic volume effect, $\omega(M)$, is given by

$$\omega(M) = CM^2 \beta \frac{dJ}{d\omega},^{19)}$$

where M is the sublattice magnetization and β a negative constant. According to the Bethe-Slater curve, $dJ/d\omega$ has a positive sign for all of the present alloys. Therefore, $\omega(M)$ should have the different sign for ferromagnetic alloys and antiferromagnetic ones and the antiferromagnetic alloys should show a volume contraction below the Néel temperature. Thus, the positive magnetovolume effect observed in antiferromagnetic alloys can not be explained by the usual mechanism based on the volume dependence of exchange interaction.

The positive magnetovolume effect observed in antiferromagnetic alloys can not be explained also by Weiss theory²⁾ which indicates the negative sign of magnetovolume effect due to the stabilization of the electronic state of the iron atom associated with smaller lattice constant as compared with the paramagnetic state.

As was discussed in the previous section, the atomic moment is induced below the magnetic transition temperature in both ferromagnetic alloys and antiferromagnetic ones. This observation suggests that the change of the atomic moment induces a volume expansion. In order to analyze phenomenologically the magnetovolume effect observed in iron and nickel, Gersdorf²⁰⁾ proposed an idea that the magnetovolume effect is attributable to the change of atomic moment.

We shall show here that the volume change due to the variation of atomic moment can be explained from the band-theoretical point of view as follows: Though the cohesive energy of $3d$ transition metals and alloys is mainly attributable to the conduction band, the contribution of $3d$ band should not be neglected. The change of $3d$ band polarization should affect the cohesive energy and this change of cohesive energy induces a variation of atomic distance. In the above mentioned discussion, we deal not with the atomic spin polarization but with the spin polarization of $3d$ band in the whole crystal. However, if one defines the atomic moment as a polarization of Wannier function at the atomic site as discussed by Bailyn¹¹⁾ one can regard the atomic moment as the $3d$ band polarization. According to this idea, disappearance of the spontaneous magnetization or of the sublattice magnetization does not imply disappearance of $3d$ polarization. Thus, the very small magnetovolume effect of iron, cobalt and nickel can be understood.

The physical origin of the magnetovolume effect caused by the change of magnetic moment is explained as follows. In the paramagnetic state where the $3d$ band is not polarized, $3d$ electrons occupy the lower parts of both up and down spin sub-bands which have mainly bonding character. If the $3d$ band polarized perfectly, the up spin band is fully occupied by electrons and the number of electrons with bonding character decreases. Then, the contribution of down spin band to the cohesive energy is reduced and the lattice constant is increased. Therefore, the volume in a magnetically ordered state becomes large as compared with that in a paramagnetic state. This effect, of course, is most remarkable in the case of the just half-filled band. We roughly estimated the order of this effect using a very simplified model. As described in Appendix, this effect causes the volume change of about 10 % in the most idealized case. The volume change of the Invar alloys, which have the largest volume effect among actual magnetic materials in $3d$ transition metals and alloys, is at most a few per cent. Considering the roughness of estimation, the agreement seems to be good. The difference between estimated value and observed one may be due to oversimplification of the model and the estimation may give the upper limit of the effect.

It should be emphasized that this mechanism should not be neglected as an origin of magnetovolume effect and is probably the dominant origin of the Invar effect and also the magnetovolume effect of antiferromagnetic FeNiMn alloys.

On this viewpoint, the following experimental facts should be noted. 1) The Néel temperature of chromium metal, which is regarded as a typical itinerant antiferromagnet, decreases remarkably by applying pressure.²¹⁾ This observation can be interpreted in terms of the proposed mechanism as follows: Theories of itinerant antiferromagnet show that there is no atomic moment above the Néel temperature and the moment is induced below the Néel temperature. This prediction was confirmed experimentally by neutron scattering.²²⁾ According to our model, this induced moment causes the volume expansion. Then, a negative pressure effect on the Néel temperature can be expected. 2) The Néel temperature of FeMn alloys which are reputed to have induced moments also remarkably decreases by applying pressure.¹⁹⁾ 3) It is well known that the Curie temperature of the Invar alloys is sharply reduced by pressure.²³⁾ As mentioned above, the atomic moment of iron atom may be remarkably induced below the Curie temperature and this change of moment may cause a large volume effect. On the other hand, it should be noted that the magnetovolume effects of b.c.c. iron, cobalt and nickel are very small.²⁴⁾ According to our model, this fact suggests that the degree of spin polarization of the $3d$ band hardly changes at the Curie temperature. This speculation contradicts to the classical band theory of ferromagnetism. However, if one interprets the spin polarization as the local one or in other words as the spin polarization of the Wannier function at the atomic site, the spin polarization does not necessary to change at the Curie temperature. Then, we may say that the permanent moment exists above the Curie temperature in these metals or in other words the localized model is good for these metals.

Acknowledgments

The authors are indebted to Dr. T. Tsuchida for many discussions and to Messrs. M. Hayase and S. Kawarazaki for their assistances of measurements of thermal expansion and electrical resis-

tivity. Their thanks are also due to Professor W. E. Wallace at University of Pittsburgh for reading the manuscript.

Appendix

In order to calculate the volume change caused by the 3d band polarization, we shall make the following assumptions :

1) The cohesive energy is mainly determined by conduction electrons. This contribution, E_c , is expressed by

$$E_c = \frac{K}{2} \omega^2,$$

where K is the bulk modulus, ω , the relative volume change given by $\Delta V/V$.

2) The contribution of 3d band to cohesive energy is expressed by the volume dependent energy, $E_{3d}(V)$, which results from the change of band width due to volume change as

$$E_{3d}(V) = \int_{-\infty}^{\infty} f E \rho_{\pm}(E, V) dE,$$

where f is the Fermi distribution function, $\rho_{\pm}(E, V)$ the state density of \pm spin band at the volume V .

3) The 3d band is simply represented by the for single band with the shape of

$$\rho_{\pm}(E) = \frac{3}{4} N \left(\frac{W}{2} \right)^{-3/2} \sqrt{-E + \frac{W}{2} + E_{\pm}}$$

for $E < E_{\pm}$,

$$= \frac{3}{4} N \left(\frac{W}{2} \right)^{-3/2} \sqrt{E + \frac{W}{2} - E_{\pm}}$$

for $E > E_{\pm}$,

where W is the band width, N the total number of 3d electrons, and E_{\pm} the middle points of \pm spin bands.

4) The exchange integral or the separation of \pm spin bands does not change with volume.

Then, the total energy can be calculated under the following conditions.

- 1) $T = 0$ K.
- 2) The 3d electrons occupy just half of the band.
- 3) $E_{\pm} = 0$ for the paramagnetic state and $E_- - E_+ > W$. These conditions are schematically shown in Fig. A.1.

It is obvious that E_{3d} does not depend upon the band width in the fully polarized state. This means that the 3d band has no contribution to the

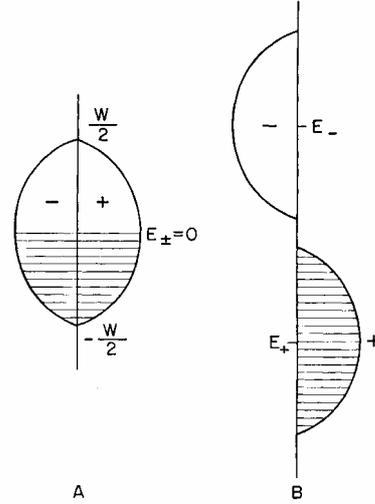


Fig. A.1. Schematic 3d band structure of Invar alloys. A indicates the unpolarized band above the magnetic ordering temperature and B indicates the completely polarized one below the magnetic ordering temperature. In both cases, electrons occupy just half of all the states.

cohesion. On the other hand, for the paramagnetic state the total cohesive energy, E_t , is given by

$$E_t = \frac{K}{2} \omega^2 + 2 \int_{-W/2}^0 E \rho(E) dE = \frac{K}{2} \omega^2 - \frac{N}{5} W(\omega).$$

The equilibrium atomic separation moves from $\omega = 0$ and is obtained by minimizing the total energy as

$$\frac{\partial E}{\partial \omega} = K\omega - \frac{N}{5} \frac{\partial W}{\partial \omega} = K\omega - \frac{N}{5} \frac{\partial W}{\partial d} \frac{\partial d}{\partial \omega} = 0$$

where d is the atomic distance given by $d = d_0(1 + \omega/3)$; d_0 is the equilibrium atomic separation determined only by the conduction electrons. Thus, the volume change due to magnetic ordering, ω , is given by

$$\omega = \frac{N d_0}{15K} \frac{\partial W}{\partial d}.$$

$\partial W/\partial d$ was estimated from the result of band calculation for copper by Krutter²⁵⁾ to be 13 erg/atomic unit. Putting $K = 14 \times 10^{11}$ dyne/cm², $N = 8 \times 10^{22}$ /cm³ and $d_0 = 2.7$ atomic unit, we can get $\omega = 10^{-1}$.

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