Electron-Phonon Interaction Mechanism of Temperature Induced Ferromagnetism

To cite this article: Shuji Ukon et al 1987 Jpn. J. Appl. Phys. 26 837

View the article online for updates and enhancements.
Electron-Phonon Interaction Mechanism of Temperature Induced Ferromagnetism

Shuji UKON*, Chikako TANAKA**, Keiko KAWABATA***, and D.J. KIM

Department of Physics, Aoyama Gakuin University, Chitosedai, Setagaya-ku, Tokyo 157, Japan

Y$_3$Ni$_7$, which is paramagnetic at T=0, becomes ferromagnetic when the temperature is raised to $\sim 7K$; then at $\sim 60K$ the system again makes a phase transition to paramagnetic state. We show how it is possible to understand such a behavior of an itinerant electron system if we take into account the effect of the electron-phonon interaction.

Recently Beille et al.[1] reported that YNi$_3$ alloy series show quite a variety of characteristically different magnetic behaviors depending upon their compositions. An interesting case is Y$_3$Ni$_7$... this system, which is paramagnetic at T=0, undergoes a ferromagnetic transition when the temperature is raised to $T_\text{c} = 7K$; then if the temperature is further raised to $T_\text{c} = 60K$, the system makes another phase transition to paramagnetic state. In the ferromagnetic state between $T_\text{c}$ and $T_\text{f}$ the spontaneous magnetization is very small, $< 0.02 \mu_B$ per Ni atom at the maximum.

The possibility of such a magnetic behavior as observed in Y$_3$Ni$_7$ was earlier noted by Shimizu [2] and Irkin [3]. As Moriya [4] recently pointed out, however, it seems very difficult to quantitatively account for the present observations on Y$_3$Ni$_7$ within those theories [2, 3, 5]. Moriya [4] applied their spin fluctuation theory on this problem, but did not succeed to offer quantitatively satisfactory analysis.

Recently we pointed out the importance of the role of the electron-phonon interaction (EPI) in itinerant electron magnetism [6]. With such effect of EPI, besides showing how the Curie-Weiss like temperature dependence can be obtained without invoking localized moment, we succeeded in reproducing observed various temperature dependence of the magnetic susceptibility of transition metals [7]. In this paper we show how the consideration of EPI makes it possible also to quantitatively understand those observations on Y$_3$Ni$_7$.

The mechanism why the EPI or phonons are relevant to magnetism is as follows. Both of the magnetic susceptibility, $\chi$, and the spontaneous magnetization, $M$, of a metal are determined from the magnetization dependence of the free energy, $F(M)$: $\chi' = \frac{\partial F(M)}{\partial M}$ and $M = 0$. The free energy of a metal consists of the contributions from electrons, $F_e$, and phonons, $F_p$. Because the phonon frequency is screened by conduction electrons and the screening behavior changes with the spin splitting of the electron bands, $F_p$ also becomes $M$ dependent. The crucial observation is that although $\frac{\partial F_p}{\partial M} = \Omega M\nu_p/\epsilon_p = 10^{-2}$, $\nu_p$ and $\epsilon_p$ being respectively the phonon Debye frequency and the electron Fermi energy, the size of changes due to $M$ is of the same order, $|\Delta F_p(M)/\Delta F_e(M)| = O(1)$. This can be easily understood by considering the energies $F_e$ and $F_p$ in place of $F_e$ and $F_p$ in a ferromagnet with Curie temperature $T_\text{f}$; the electron energy, $|\Delta F_e(M)|$, gained by a full magnetization is $\sim N\mu_B^2$, $N$ being the number of electrons or ions. As for phonons, for $T = 0$, $F_p = N\mu_p^2$. Since by the full splitting of the bands the size of the screening constant, which is proportional to the electronic density of states at the Fermi surface, changes by one order of magnitude, $|\Delta F_p(M)| = N\mu_p^2 = N\nu_p^2\theta_D^2$, $\theta_D$ being the Debye temperature. Since generally $\theta_D$ and $\mu_p$ are of the same order, $|\Delta F_p(M)| = |\Delta F_e(M)|$.

With such consideration of EPI effect, and by using the Debye approximation for phonons, we obtain the paramagnetic susceptibility in the following form [6].

$$\chi = 2\pi \frac{F(0)}{N(0)} [1 - (\nu F_e)^2]$$

(1)

where $\nu$ is the exchange interaction between electrons, and

$$F(0) = N(0) \left[ 1 - \frac{1}{6} \left( \frac{N'(0)}{N(0)} \right)^2 - \frac{N'(0)}{N(0)} \right] \frac{\nu}{2\theta_D^2}$$

where $N(0)$, $N'(0)$, and $N''(0)$ are the electronic density of states and its energy derivatives at the Fermi level.

The effect of EPI on $\chi$ is given by

$$\chi_p F(0) = \frac{L}{T\theta_D} \frac{L}{2N(0)} \frac{L}{2N'(0)} \left[ 1 - \frac{N'(0)}{N(0)} \right] \left[ 1 - \frac{N'(0)}{N(0)} \right]$$

(2)

where $W$ is the width of electron energy band introduced to make $L$ dimensionless, $W = \frac{N(0)}{2N(0)} \left[ 1 - \frac{N'(0)}{N(0)} \right] \left[ 1 - \frac{N'(0)}{N(0)} \right]$.

$P(T/\theta_D) = 3/8 + (T/\theta_D)D(\theta_D)/T$.

(4)

where $D(x)$ is the Debye function; as shown in Fig.3(a), $P(T/\theta_D) = T/\theta_D$ for $T < 3/8$, and $P = 3/8$, for $T > 3/8$.

The principal problem is to see whether it is possible at all for the $\chi$ of eq. (1), which is positive at $T=0$, to become first negative at $T = 7K$ and then to become positive again for $T = 60K$ after such a small temperature increase. The quantity $L$, which determine the size of the phonon effect, can be calculated if $N(\epsilon)$ near the Fermi surface and $V$, or $V = N(\epsilon)$ are given. In the present analysis we use the $N(\epsilon)$ of Fig. 1(b) which is obtained by approximately fitting to the band calculation result of ref. 5 by a polynomial near the Fermi level. In Fig. 1(a), $V = 0$ is calculated for different values of $V$ by changing the location of $\epsilon_c$. We put $W = 0$, $L$ depends very sensitively on the value of $V$ and $\epsilon_c$.

In obtaining the result of Fig. 2, we chose the location of the Fermi level as indicated by the
arrow in Fig. 1(b), which is very close to the result of ref. 5, and we assumed $\nu = 0.9607$ and $T_c = 100K$. In this way we obtain the magnetic susceptibility of Fig. 2. $\chi$ diverges at $T = 19K$ and $T_c = 70K$. Although the values of $T_c$ and $T_p$ are slightly different from the observed values, the general feature of our result is very satisfactory; note that even the increase of $\chi$ toward $T = 0$ is reproduced.

An analysis how such result was obtained is given in Fig. 3. According to eqs. (1)-(3), the temperature dependence of $\chi$ is determined by that of $F(0), P(T)$, and $L$. The temperature dependence of $L$ comes from $\Phi F(0)/(1 - \Phi F(0))$, which is actually that of the Stoner susceptibility, in the last term of eq. (3). First in Fig. 3(a) we show the temperature dependence of $\Phi F(0)/(1 - \Phi F(0))$ for two slightly different values of $\nu$ but for the same common electronic state of Fig. 1(b), and that of $P(T)$. Then in Fig. 3(b) we show the corresponding temperature dependence of $(\nu + 1)F(0)$. It is surprising that a slight difference in the behaviour of $\Phi F(0)/(1 - \Phi F(0))$ in Fig. 3(a) brings about such a qualitative difference in the final result. Note that the slight increase toward $T = 0$ of $(\nu + 1)F(0)$, which is responsible for the corresponding increase in $\chi$, is caused by the temperature dependence in $F(0)$.

We calculate also the magnetization between $T_c$ and $T_p$ by the same approximation as shown in Fig. 2. The obtained magnetization is about half of the observed one.

In conclusion, our present result strongly indicates the importance of considering the role of the electron-phonon interaction in understanding magnetism of metals.

REFERENCES
3) Yu.P.Irkin: JETP Lett. 23 (1971) 116

Fig. 1. L for various values of $\nu$ is calculated in (a), as the function of the location of the Fermi energy in the electronic density of states of (b). The arrow indicates the location of the Fermi level and we put $\nu = 1$. 0 eV.

Fig. 2. Magnetic susceptibility (broken line) and magnetization (solid line) calculated for the electronic density of states of Fig. 1(b) with $\nu = 0.9607$ and $\theta_p = 100K$.

Fig. 3. In (a) is shown the temperature dependence of $\Phi F(0)/(1 - \Phi F(0))$ and $P(T/\theta_p)$ for the same situation as in Fig. 2 except that as for the former besides the case of $\nu = 0.9607$ (solid line) also is shown the case of $\nu = 0.95$ (broken line). In (b), the arrows show at what temperatures the ferromagnetic transition occurs.