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SPIN POLARIZATION AROUND A LOCALIZED MAGNETIC IMPURITY IN A MAGNETIZED METAL

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Recently, neutron diffraction experiments[1] have been used to obtain the spatial distribution of the magnetic disturbance about solute atoms in Pd, Ni, and Fe. These measurements show that the disturbance produced around a magnetic impurity is quite different for different host metals. For low-concentration Pd:Fe alloys, the range of the conduction-electron polarization about the Fe impurity is long—on the order of 10 Å. In contrast to this long-range behavior, the disturbance due to a magnetic impurity in ferromagnetic Ni is almost confined to the impurity site. A magnetic impurity in ferromagnetic Fe produces a disturbance intermediate in range between Pd:Fe and Ni. In this Letter we present calculations which correlate the behavior of the disturbance associated with a localized moment with the band splitting of the host-metal electrons including exchange effects fully. We find that the range and amplitude of the polarization produced by a magnetic impurity are very sensitive to the spin splitting of the host-metal band. The range is large for small magnetization (dilute Pd:Fe) and on the order of an atomic distance for nearly complete magnetization (a magnetic solute atom in ferromagnetic Ni where one spin band appears to be full).[2] Furthermore, in dilute Pd:Fe alloys we can account for the sharp concentration-dependent decrease of the magnetic moment per Fe atom[3] by considering the increase in the splitting of the host Pd bands caused by adding Fe impurities.[4]

Although Low and his collaborators' experiments cover more complicated situations, we consider those situations in which an impurity forms a localized moment and calculate the spin polarization about the impurity.

This problem has two aspects. The first is the formation of the localized magnetic state on the impurity site, and the second is the spin polarization around the impurity.[5,6] In this paper we concentrate our discussion on the second aspect of this problem.

Our problem may be simplified without losing any essential features by replacing the effect of an impurity spin with an effective δ-function magnetic field $H\delta(r)$,[7] where we assume that the site of the impurity is at the coordinate origin. The conduction-electron spin polarization $\sigma(\vec{r})$ around the impurity is given as

$$\sigma(\vec{r}) = H\frac{1}{(2\pi)^3}\int \chi(\vec{q})e^{i\vec{q}\cdot\vec{r}}d\vec{q}, \qquad (1)$$

where $\chi(\vec{q})$ is the wave-number-dependent susceptibility of the host metal.

We adopt a single-nondegenerate-band model[8] for the transition metals, and for simplicity replace the actual Coulomb interaction by a δ-function interaction in which the Fourier transform is a constant, v. For a paramagnetic metal like pure Pd, or Fe and Ni above their Curie temperatures, the exchange-enhanced susceptibility $\chi^p(q)$ obtained using the random phase approximation is $\chi^p(q)=\frac{1}{2}(g\mu_B)^2F(q)[1-vF(q)]^{-1}$, where

$$F(q)=-\sum_k(f_k-f_{k-q})(\epsilon_k-\epsilon_{k-q})^{-1};$$

ϵ_k is the one-particle energy of a conduction electron with momentum $\hbar k$, f_k the Fermi distribution function, μ_B the Bohr magneton, and g the electronic g factor. In a free-electron model where $F(q)$ decreases with increasing q, the exchange-enhanced $\chi^p(q)$ is larger for smaller q and therefore the range of $\sigma(\vec{r})$ is enhanced.[9] Numerical calculations have shown that when $vF(0)$ is very near 1, this effect is especially significant, and the long-range polarization observed in Pd is attributed to this effect. Recently, Clogston[10] has demonstrated the additional importance of interatomic electron interaction in Pd. If we consider the finite range of the interaction, the v appearing in the equation for $\chi^p(q)$ becomes effectively q dependent. This fact causes an even more rapid decrease of $\chi^p(q)$ with increasing q, and accordingly contributes to make the range of the magnetic disturbance longer.

The main difference between pure Pd and the ferromagnetic metals (Fe or Ni or Pd:Fe alloys) is that in the latter the host-metal electron systems have a spontaneous magnetization below their Curie temperatures. In the presence of a spontaneous magnetization, the relevant component of the susceptibility tensor which should appear in the integral for $\sigma(\vec{r})$ of Eq. (1) is[11]

$$\chi_{zz}(\vec{q})=\tfrac{1}{4}(g\mu_B)^2\left[\frac{F_+(\vec{q})+F_-(\vec{q})+2vF_+(\vec{q})F_-(\vec{q})}{1-v^2F_+(\vec{q})F_-(\vec{q})}\right], \quad (2)$$

where we assume that the spontaneous magnetization is along the z axis and where

$$F_\pm(\vec{q})=-\sum_k\frac{f_{k\pm}-f_{k-q\pm}}{\epsilon_k-\epsilon_{k-q}}. \quad (3)$$

It is easy to see that if there is no magnetization, namely when $f_{k+}=f_{k-}$, $\chi_{zz}(\vec{q})$ reduces to $\chi^p(q)$ and the usual arguments for the range of $\sigma(r)$ apply. When the host is magnetized, however, $\chi_{zz}(\vec{q})$ and $\chi^p(q)$ are quite different.

We have numerically calculated the integral for $\sigma(\vec{r})$ using Eq. (2) for $\chi(q)$ as a function of the relative magnetization of the host metal, $p=(n_+-n_-)/2n$ where $n_\pm$ are the number of electrons (holes) for each spin and $2n$ is the total number of electrons (holes). To simplify the calculations we have introduced the following approximations: (i) The host-metal d electrons (d holes in Pd, Ni, and Fe) are represented by a parabolic band,[8] where $n_\pm=k_{F\pm}^3/6\pi^2$ and $n_++n_-=2n$ is a constant, $k_F^3/3\pi^2$. (ii) We have neglected the temperature dependence of the function $F(q)$.[12] For the parabolic band $F_\pm(q)$ is given by

$$F_\pm(q)=N(0)_\pm\left[1+\frac{1-x_\pm}{2x_\pm}\ln\left|\frac{1+x_\pm}{1-x_\pm}\right|\right],$$

where

$$N(0)_\pm=mk_{F\pm}/2\pi^2;\quad x_\pm=q/2k_{F\pm}.$$

In the calculations which follow we have chosen $vN(0)=1$ (the Stoner condition for ferromagnetism),[13] where $N(0)$ is the density of states at the Fermi surface per spin of the host metal in the paramagnetic state. In Fig. 1, $\sigma(r)$ is plotted for various values of the relative magnetization of the host metal for a typical value of $k_F=10^8$ cm^{-1}. The range and magnitude of the magnetic disturbance turns out to be very large for a small polarization of the host metal. In addition to the numerical calculation plotted in Fig. 1, we estimate the asymptotic behavior of the $\sigma(r)$ integral for large r by expanding the denominator of the right-hand side of Eq. (2) in q and retaining terms to order $(q/k_{F\sigma})^2$, obtaining $\sigma(r)\propto e^{-\kappa r}/r$, where

$$\kappa^2=\frac{1-v^2N_+(0)N_-(0)}{(v^2/12)(k_{F+}^{-2}+k_{F-}^{-2})N_+(0)N_-(0)}; \quad (4)$$

κ^{-1} may serve as a reasonable measure for the range of the spin polarization. In Fig. 2 we plot $\kappa^{-1}k_F$ as a function of the relative magnetization of the host metal. In addition we have also included the relative magnitude of $\sigma(r)$ at $r=1$ Å as a function of relative magnetization.

In ferromagnetic Ni it is supposed that one

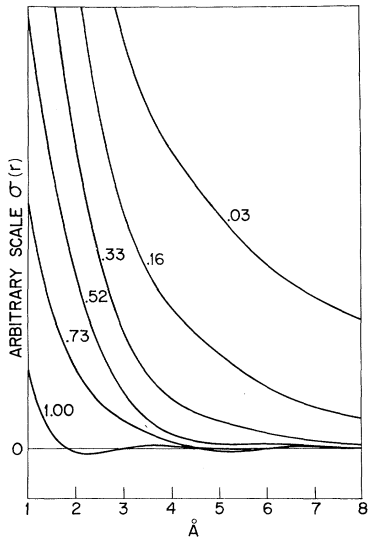

FIG. 1. Plot of $\sigma(r)$ vs r for various values of the relative magnetization p. The range is very large for small p (i.e., the $p=0.03$ curve does not change sign until $r \simeq 240$ Å). The $p=1$ curve is just the simple Ruderman-Kittel-Kasuya-Yosida oscillation ($k_{F+}=2^{1/3} \times 10^8$ cm^{-1}) and may serve as a reference level for comparison.

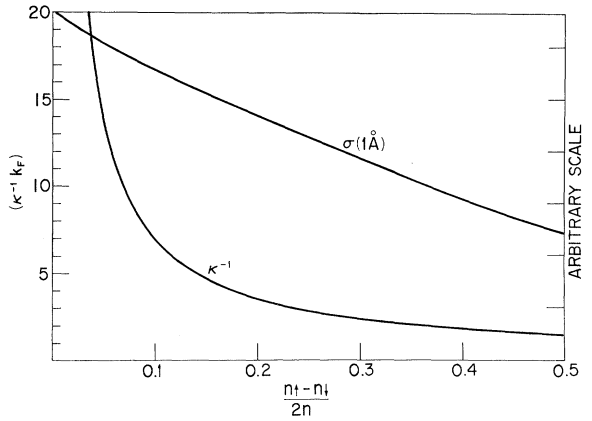

FIG. 2. Plot of the "range" as defined by Eq. (4) as a function of the relative magnetization (left-hand coordinate) and the relative amplitude of $\sigma(r)$ at $r=1$ Å (right-hand coordinate) in the interval $0 \leq p \leq 0.5$. For small values of p the range is a very rapidly decreasing function of the relative magnetization.

spin d band is completely filled, $p \simeq 1$.[2] In such a situation Eq. (2) reduces to $\frac{1}{4}(g\mu_B)^2 F_+(q)$ and with this expression for $\chi(q)$ the integral in Eq. (1) gives the simple Ruderman-Kittel-Kasuya-Yosida oscillations without any exchange-enhancement effects. This tendency is also seen from Figs. 1 and 2 and this fact seems to explain the experimentally observed short range for the disturbance produced by a magnetic impurity in ferromagnetic Ni.

In ferromagnetic Fe both up- and down-spin bands are supposed to be partially filled[2,14] which represents an intermediate value for the relative magnetization. This explains why the range of the magnetic disturbance in Fe is appreciably larger than in Ni.

The case of dilute Pd:Fe alloys below their Curie temperatures corresponds to the situation of small relative magnetization, $p \ll 1$, and therefore the range is very long. As we increase Fe concentration, the Pd spin bands split on the average to an effectively higher relative magnetization p and thus the range, and accordingly the total magnetic moment per Fe atom, decreases.[1,3]

From the analysis above we can naturally propose the following experiment: to perform neutron-diffraction experiments on magnetic impurities in ferromagnetic Ni and Fe as a function of temperature. As the temperature increases, the spin splitting of the bands is reduced, and we might expect to see a significant increase in the range of the polarization around a magnetic impurity. This is essentially what happens when the Fe concentration is decreased in Pd:Fe alloys.

Our calculations may be extended by including the effects of the finite range of the electron interaction as well as the details of the actual band structure in transition metals. By including the q dependence of the electron interaction, the denominator on the right-hand side of Eq. (4) becomes smaller[10] and thus increases the sensitivity of the range to the relative magnetization. Recent band calculations show that the Fermi levels in paramagnetic Ni, Fe, and Pd[2,14] lie close to the peaks in the density of states. Near these peaks the product $N_+(0)N_-(0)$ in Eq. (4) decreases more rapidly with increasing relative magnetization than is the case for simple parabolic bands, thus amplifying the effects we have considered.

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[12]Thus, in reality, the density of states in the following discussions should be interpreted to be $F_\pm(0)$ which is related to the former by

$$F_\pm(0) = \int N_\pm(\epsilon) \frac{\partial f_\pm}{\partial \epsilon} d\epsilon,$$

or, for the parabolic band

$$F_\pm(0) = N_\pm(0)\left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\epsilon_{F\pm}}\right)^2 + \cdots\right].$$

[13]More precisely, $vF(0)_{T=T_c} = 1$. This condition is not satisfied in pure Pd where $vN(0) \simeq 0.9$. In Ni and Fe, $vF(0)$ may be greater than 1 below the Curie temperature. As can be easily shown, these details do not affect the qualitative features of our problem.

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EVIDENCE OF HOLE-OPTICAL-PHONON INTERACTION IN DEGENERATE SILICON IN TUNNELING MEASUREMENTS†

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Tunneling from a metal into degenerate p-type silicon exhibits peaks in d^2i/dV^2 at biases $eV = \pm\hbar\omega_0$, where $\hbar\omega_0$ is the $k = 0$ optical-phonon energy of the semiconductor. It is suggested that these peaks reflect modifications in the bulk semiconductor states at energies $\hbar\omega_0$ above and below the Fermi energy arising from hole–optical-phonon interaction. An additional peak near the optical-phonon frequency, but well resolved from it, is identified with vibrations of the boron acceptor impurity.

Interaction of holes with optical phonons in the covalent group-IV semiconductors was originally inferred from analysis of the temperature dependence of the hole mobility[1,2] and has recently been more directly verified by observations of oscillatory photoconductivity[3] in germanium[4] and silicon.[5] In the present measurements of d^2i/dV^2 characteristics of metal-insulator-semiconductor tunnel junctions, formed using indium on degenerate p-type silicon, the interaction of holes and optical phonons at small wave vector k is clearly indicated by peaks occurring at values of the applied bias voltage V such that $eV = \pm\hbar\omega_0$, where $\hbar\omega_0$ is the optical phonon energy at $k = 0$. The absence of strong zone-boundary phonon effects[6] is consistent with a direct tunneling process from the metal Fermi surface to a small Fermi surface in the semiconductor valence band at $k \cong 0$. The behavior at positive bias $eV = +\hbar\omega_0$, corresponding to a positive step in conductance, resembles that observed in direct tunneling