

Magnetic-nonmagnetic transition in Ti-Mn alloys

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As the concentration of the magnetic component (Mn) in titanium is increased, the average magnetic moment of the impurity ions decreases, vanishing at ~ 10 at. % Mn. The concentration dependence of the magnetic moment is found.

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Only manganese and chromium ions among the $3d$ -metal ions are magnetic-moment carriers when impurities in titanium.^{1,2} It has been found that the temperature-dependent contribution to the magnetic susceptibility from the magnetic moments of the manganese and chromium ions disappears at concentrations of these impurities below 10 at.%. The alloys exhibit absolutely no evidence of a magnetic ordering in this composition range. This behavior is at odds with the customary evolution of the magnetic state of alloys, according to which an increase in the concentration of the magnetic component gives rise to a magnetic order in the alloy. The concentration dependence of the magnetic moment of impurity ions in titanium is thus quite interesting. In this letter we report a study of this dependence for the alloys $\text{Ti}_{1-x}\text{-Mn}_x$ ($0 < x \leq 0.1$), and we report observation of a magnetic-nonmagnetic concentration transition, where the transition is a change in the magnetic state of the manganese ions.

Figure 1 shows the concentration dependence of the effective magnetic moment per manganese ion. The moments were calculated from measurements of the temperature dependence of the magnetic susceptibility carried out in a magnetic field $H = 35$ kOe over the temperature range 4.2–300 K.

With increasing manganese concentration in the titanium (Fig. 1), the magnetic

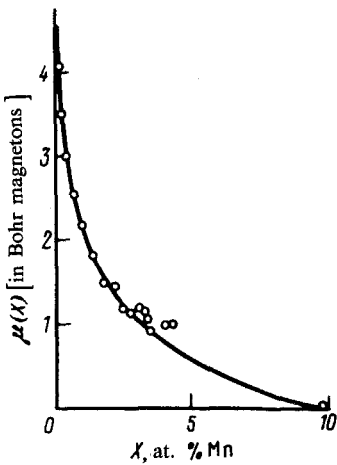


FIG. 1. Concentration dependence of the effective magnetic moment of the manganese ion in Ti-Mn alloys.

moment of the manganese ions falls off rapidly, vanishing at $x \approx 0.10-0.12$. We are thus seeing a magnetic-nonmagnetic transition with increasing concentration of the magnetic component. We wish to call attention to some features of the curve in Fig. 1: a) In the limit $x \rightarrow 0$ we find $\mu(x) \rightarrow 5\mu_B$, where μ_B is the Bohr magneton, so that in the "one-impurity limit" the manganese impurity has an integer spin configuration, $s = 2$; b) the $\mu(x)$ curve is concave toward the coordinate axes; c) the magnetic moment vanishes at $x \approx 0.10-0.12$. With $z = 8$ nearest neighbors, this result corresponds approximately to the condition $zx \approx 1$, under which one more impurity atom enters the nearest-neighborhood sphere of the impurity atom.

Analysis of the possible reasons for this behavior of the magnetic moment leads to the conclusion that the most likely reason for the disappearance of the magnetic moment is an overlap, which increases with increasing concentration, of the wave functions of the electrons belonging to different impurity atoms. This overlap ultimately causes a delocalization of the impurity $3d$ states and gives rise to an impurity d band (this possibility was first pointed out by Friedel³).

In this case the degree of localization of an electron at an impurity site is determined by a competition by the "impurity-impurity" transport integral $I(R)$ (R is the average distance between impurities) and the Coulomb correlation energy at the site, U . We thus have⁴

$$\mu(R) \sim [1 - zI^2(R) / U^2], \quad (1)$$

For wave functions which fall off with distance in proportion to $\exp(-2\alpha R)$, the asymptotic behavior of $I(R)$ is

$$I(R) = I_0 \exp(-\alpha R). \quad (2)$$

Estimating the average distance between impurities from $R \approx (3/4\pi)^{1/3} a / (zx)^{1/3}$, substituting this estimate into (2), and then substituting the result into (1), we find the concentration dependence of the magnetic moment to be

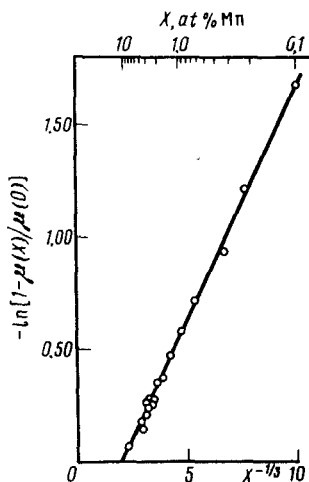


FIG. 2.

$$\mu(x) = \mu(0) \left\{ 1 - \frac{zI_0^2}{U^2} \exp[-0.31 \alpha a / x^{1/3}] \right\}, \quad (3)$$

where a is the lattice constant.

Figure 2 shows the results of an analysis of the experimental magnetic moments by means of expression (3). As $\mu(0)$ we adopted the theoretical value⁵ $4.9 \mu_B$ for the magnetic moment of manganese for an $s = 2$ spin configuration; this value agrees well with the value which we found for μ in the "one-impurity limit." We see a good agreement between the concentration dependence predicted by (3) and the measured magnetic moments over a broad concentration range (two orders of magnitude).

To the best of our knowledge, a magnetic-moment dependence of the type in (3) has not previously been discussed in the literature. It is thus naturally interesting to compare this expression with experimental results obtained for other systems of this type. One way to test the physical justification for using expression (3) to analyze experimental data, however, might be to estimate the delocalization radius α^{-1} of the d wave functions of manganese. We can do this by working from the slope of the line in Fig. 2. We find $\alpha^{-1} \approx 1.6 d$: a value which is completely reasonable from the physical standpoint.

We wish to emphasize the two most important conclusions that follow from these results. 1) In the limit of very dilute alloys, a manganese impurity in titanium has an ion configuration with an integer spin. It follows that the broadening of the impurity d states due to mixing with states from the conduction band of the matrix is anomalously slight (if it occurs at all). 2) The fact that the dependence $\mu(x)$ is described well by expression (3) means that the degree of broadening of the impurity states is a function of only (or of nearly only) the average distance between impurity atoms, as it would be if two metal atoms approached each other in a vacuum (a Mott transition⁴).

In summary, these results indicate that the states of the matrix conduction band

and the impurity d states act as autonomous electron subsystems in these alloy systems. This circumstance is apparently a governing factor in the evolution of the electron spectrum of the alloys as the composition is varied.

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