

transition may tend to sharpen and may become first-order as in the Bean-Rodbell model. This type of procedure has been used to explain thermal expansion effects in an itinerant electron AFM³⁴ where only the electron-lattice interaction was considered. In this case it was demonstrated that the balance set up between the elastic and electron-lattice forces is important in explaining the anomalous behavior of the thermal expansion for temperatures near T_N . However, for the parameters used in the theory, no first-order nature was observed in the phase transition.³⁴ It is anticipated that inclusion of exchange-striction effects could precipitate a first-order phase transition for the itinerant electron AFM.

Unpublished x-ray data by Goodenough³⁵ on $\text{MnAs}_{0.80}\text{Sb}_{0.20}$ show that the unit cell volume is quite temperature dependent for temperatures near T_c where the volume decreases continuously from a value of $70.81(\text{\AA})^3$ at a temperature of approximately 100°K below T_c to a value of approximately $70.19(\text{\AA})^3$ at T_c . This represents approximately a 0.9% decrease in the volume. For MnAs there is approximately a 1.8% discontinuous volume decrease at T_c for increasing temperature. It is therefore apparent that for $x \gtrsim 0.80$ there are large interactions of the lattice with the exchange energy and/or the electronic energy. The volume changes associated with these interactions depend on the magnetization. Due to the coupling, a discontinuous change in the unit cell volume is reflected in a discontinuous change in the magnetization, and vice versa.

The physical picture we have for the results of the coupling of the magnetization and the lattice is as follows. At low temperatures the magnetization takes on its saturation value, and the magnetic characteristics are determined by the bandwidth W , density of states $N(\epsilon_F)$ and the exchange

interaction I . As the temperature is increased the lattice expands, and due to electron-lattice coupling and exchange-striction, W decreases and I can either increase or decrease depending on the sign of $\partial \ln I / \partial \ln V$. For the material under consideration here, as W decreases, T_c will increase and the magnetization for $T \ll T_c$ will increase over the value it would have had if W and I did not depend on the volume. However, due to the electron-lattice and exchange-striction effects, the lattice contracts for $T \lesssim T_c$ and thus W increases and T_c decreases. Hence depending upon the amount of coupling, the rate at which W increases (or the apparent T_c decreases) determines whether the transition will be second or first-order. For the first-order transition, in the words of Bean and Rodbell,²⁷ ". . . this situation is like that of a man who has run beyond the brink of a cliff; there is no gentle way down." The critical volume discussed by Goodenough and Kafalas⁶ appears to be intimately related to the electron-lattice and exchange-striction effects as a detailed theory should show.

Finally, the rather large changes in T_c with pressure for the first-order region are noteworthy. As shown in Fig. 4 there is a discontinuous change in $\partial T_c / \partial P$ at the composition which demarcates the boundary between the first and second-order regions. In addition, there are strong hysteresis effects in the first-order region. At this time, we can offer no concrete explanation of the rather large $(\partial T_c / \partial P)$'s for the first-order region except to say that the large pressure effects appear to be connected to a "critical volume"⁶ and consequently to the electron-lattice and exchange-striction effects.

We conclude that for the first-order region electron-lattice and exchange-striction effects are important, and that inclusion of these effects in an itinerant FM model (which is in a similar spirit to the Bean-Rodbell model) will be able to explain in some detail the magnetic and structural behavior.