Unambiguous dependence of the period of the helicoidal magnetic structure in heavy magnetic rare-earth materials on the ratio *c/a* of the crystal lattice; possible association with an electron topological transition

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The period of the helicoidal magnetic structure in the magnetic rare-earth elements Tb, Dy, Ho, and Er is determined unambiguously by the ratio c/a of the hexagonal crystal lattice of these metals. The particular shape of this dependence can be explained by assuming that an extreme diameter of the Fermi surface, which determines the helicoid period according to Dzyaloshinskiĭ, undergoes a square-root singularity at $(c/a)_{cr} = 1.582$ as the result of an electron topological transition.

Heavy magnetic rare-earth materials have been the subject of active research for more than thirty years,[1–3] but there is still some question about the nature of the helicoidal (spiral) antiferromagnetic structures which are realized in some of them (Tb, Dy, Ho, Er, and their alloys with each other, Gd, Y, etc.).[3]

An exchange interaction occurs in these metals because of conduction electrons (the RKKY interaction). All these materials have very similar physical properties—so similar that these materials might be thought of as modifications of the same entity. In particular, all have an *hcp* lattice, and the lattice constants are approximately the same.

The circumstances under which the helicoidal structure forms are varied. In Tb, Dy, and Ho this structure arises with the magnetic order at the Néel temperature T_N and later converts (in a first-order phase transition) into a ferromagnetic phase at $T_1 < T_N$. In Dy, for example, we have $T_N = 179$ K and $T_1 = 85$ K, while in Tb we have $T_N = 230$ K and $T_1 = 219$ K. Alloys of these elements with yttrium behave in a similar way. At a Y concentration above a certain level, a helicoid exists down to extremely low temperatures. The period of the helicoid increases smoothly with decreasing temperature. The anomalies associated with a commensurability of the lattice and the helicoid are small (if they exist at all[4]).

In Er, in contrast, a helicoidal structure is realized only at low temperatures, $T < T_1 = 20$ K.

As the temperature is varied, changes of course occur in the lattice constants also. However, the existence of a helicoidal structure does not disrupt the lattice symmetry, which remains hexagonal.[2]

Figure 1 shows a family of curves of the helicoid rotation angle α [which is proportional to the reciprocal of the period and also proportional to the wave vector of

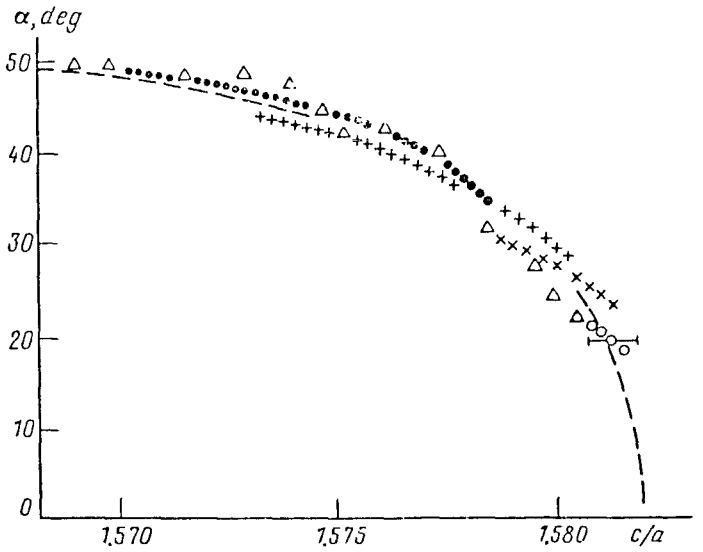

FIG. 1. The helicoid angle α versus the ratio c/a of the crystal lattice. ●—Ho; + —Dy; ×—the alloy $Tb_{0.91}Y_{0.09}$; ○—Tb; △—Er over the entire range in which a helicoid exists; ◇—various Tb_xY_{1-x} alloys at their Néel temperatures.

the helicoid, k_H: $k_H = (2\pi/c)\cdot(2\alpha/360°)$] versus the ratio c/a of the crystal lattice, for all four of these elements and also for the alloy $Tb_{0.91}Y_{0.09}$. These data are from Refs. 1–3. (Experimentally, both of these parameters are functions of the temperature, but the temperature has been eliminated from this figure. As the temperature decreases, the ratio c/a increases.) The dependence in the case of Er reduces to a single point (in the region in which a helicoid exists in it, its parameters remain nearly constant). Also shown here are the helicoid angles in various Tb–Y alloys at their Néel temperatures.

We see that all these results conform, within the experimental errors, to a common smooth curve (the dashed line).

Despite the variety of temperature intervals in which the helicoidal structures exist in the heavy magnetic rare-earth materials, the helicoid period is determined unambiguously by the ratio c/a of the crystal lattice—and by nothing else.

Here is our explanation. The period of the helicoidal structure should be determined unambiguously by the properties of the RKKY interaction. This interaction, however, is determined exclusively by the shape of the Fermi surface of the given metal. Since the structure of the outer electron shells is the same for all the heavy magnetic rare-earth materials, the shape of the Fermi surface should in turn be determined unambiguously by the ratio c/a. There should thus be an unambiguous relationship between c/a and the helicoid lattice. (These arguments tell us nothing about the conditions under which the helicoid structure actually exists. That is a considerably more complicated question, which we will not go into here.)

The data on alloys of the heavy magnetic rare-earth materials also confirm that the behavior in Fig. 1 is universal. For example, we know that as the yttrium concentration is raised in alloys of Tb, Dy, Er, and Ho with Y, the helicoid angle α increases monotonically, tending toward 50° (Ref. 3). It can be seen from Fig. 1 that this is the dependence which we would expect: The value corresponding to pure yttrium ($c/a = 1.569$) is precisely $A = 50°$. In all these alloys, the value of c/a is larger, and the helicoid angle should be smaller.

It is also known that an antiferromagnetism (i.e., a helicoid) is not realized in Tb–Gd alloys at a gadolinium concentration above 6 at. %, in Dy–Gd alloys at a gadolinium concentration above 50 at. %, or in Gd–Y alloys at a gadolinium concentration above 63 at. % (Ref. 3). The ratio c/a for gadolinium in its paramagnetic phase is[3] 1.590, i.e., considerably larger than $(c/a)_{cr}$. It is easy to see that in all these systems the value of c/a at the threshold gadolinium concentration (in the paramagnetic phase) is 1.582 ± 0.0005, i.e., the same as $(c/a)_{cr}$. (In alloys of heavy magnetic rare-earth materials with each other and with yttrium, the lattice constants are linear functions of the concentrations of the components.) This picture agrees completely with the assumption that a helicoidal structure is never realized at $c/a > (c/a)_{cr}$.

All the experimental results thus indicate that the behavior of the helicoid angle as a function of the parameter c/a is universal for all three heavy magnetic rare-earth materials and their alloys. What is the physical nature of this dependence?

We recall that the helicoid angle varies by a factor of several units as the ratio c/a changes by less than 1%. The sharpness of this variation and its overall nature suggest an electron topological transition at $(c/a)_{cr} = 1.582$ and a characteristic square-root singularity associated with this transition.[5] Calculations[6,7] of the Fermi surface of the heavy magnetic rare-earth materials (no direct experimental data are available) show that a neck-rupture transition of this sort may indeed occur (a "ribbon singularity" is ruptured). The neck exists at the lower values of c/a.

According to Dzyaloshinskiĭ,[8] the wave vector of the helicoidal structure, k_H, should be equal to one of the extreme diameters of the Fermi surface. In the heavy magnetic rare-earth materials, the transverse diameter of this ribbon singularity is presumably one such diameter.[7] When the rupture occurs, this diameter should vary as $(\epsilon_{cr} - \epsilon_F)^{1/2}$, where ϵ_F is the Fermi energy, and ϵ_{cr} is its critical value. Under the assumption that ϵ_F and ϵ_{cr} depend linearly on c/a, we find $k_H \propto [(c/a)_{cr} - c/a]^{1/2}$ in a first approximation.

According to Dzyaloshinskiĭ, the helicoid wave vector k_H and the helicoid angle α should undergo a square-root anomaly near the transition as the parameter c/a is varied. This should happen on the side on which the neck exists, i.e., at the lower values of c/a. This is the behavior we see in Fig. 1.

On the other hand, there is the conventional phenomenological approach which explains the existence of a helicoid exclusively in terms of a competition among exchange interactions between nearest moments, between next-nearest moments, and so forth.[2] That interpretation, however, cannot explain the sharp dependence of the helicoid angle on c/a. It would be difficult to accept the proposition that the RKKY exchange constants, which are determined in an integral manner by all the conduction

electrons, vary by a factor of several units (as they would have to in order to explain the observed change in the angle α) as the ratio c/a changes by less than 1%.

We draw the following conclusions. The period of the helicoidal magnetic structures in the heavy magnetic rare-earth materials is indeed determined unambiguously by the extreme diameter of the ribbon singularity at the Fermi surface. This diameter is itself determined by the ratio c/a of the crystal lattice, and it undergoes a square-root singularity associated with an electron topological transition at $(c/a)_{cr} = 1.582$. This singularity is reflected by the same singularity on the plot of the helicoid angle versus c/a.

In summary, we have found support for Dzyaloshinskiĭ's conclusions for heavy magnetic rare-earth materials—support which is slightly less indirect than that which has existed before now. If the conclusions reached in this study are correct, then magnetic rare-earth materials are the first examples of entities in which an electron topological transition not only is reflected in kinetic properties but also unambiguously determines the magnetic structure.

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