MAGNETIC PROPERTIES OF METALS. IV. PURE ZINC AND SOLID SOLUTIONS OF MAGNESIUM IN CADMIUM

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The monotonic part of the magnetic susceptibility of zinc and cadmium alloys containing up to 10 at.% magnesium is investigated at temperatures between 4.2 and 300°K. Diamagnetism maxima were observed in pure zinc at 112°K and in cadmium alloys containing 0.5 and 6.5 at.% of magnesium at 4.2°K; these correspond to band singularities passing near the Fermi surfaces. This yielded the band splitting and relevant parameters of the effective lattice potential V and spin-orbit interaction Δ_K. For zinc (at 112°K) $V_{100} = -0.0063$ Ry and for cadmium (containing small amounts of magnesium) $V_{100} = -0.006$ Ry and $\Delta_K = 0.007$ Ry.

THE experimental data on the dimensions of the Fermi surface yield the individual Fourier components of the effective lattice potential, which is an important characteristic capable of describing a majority of the properties of transition metals.[1] This source of information concerning the lattice potential is confined to pure metals and requires computer calculations. Under favorable conditions, however, there can appear near the Fermi level E_F singular values of the band energies, so that their relative placement can be easily changed by different actions. The passage of the singular points of the bands past the Fermi level, accompanied by a change in the topology of the Fermi surface, can be observed by determining the singularities of the electronic characteristics.[2] Inasmuch as the special values of the energy correspond essentially to symmetry points of the bands, their position can be easily expressed with the aid of the Fourier components of the effective potential V_{ikl}, and the latter can be obtained from the Fermi energy, which is used as a reference, and from the character of the employed action. In this paper we present the results of a realization of such a program for pure zinc and for solid solutions of magnesium in cadmium. The sensitive indicator of the passage of the singular points of the bands past the Fermi level was the monotonic part of the magnetic susceptibility.

CHARACTERISTICS OF THE INVESTIGATED OBJECTS

Zinc and cadmium are divalent metals with hexagonal close-packed lattice, but with a period ratio c/a which greatly exceeds the ideal value. The Fermi level for the empty lattice with such a structure is close to the energy at the point K—at the midpoint of the vertical edge of the Brillouin zone, where the bottom of the electron band is in contact with two hole bands (the designation of the symmetry points and of the levels in accordance with their irreducible representation is that of [3], and the level energies are designated in the same manner as the levels themselves). The lattice potential splits the triply degenerate level K into two (Fig. 1) with energy (neglecting the influence of the higher levels and the spin-orbit interaction)

$$K_1 = K - V_{100},$$
$$K_5\ (\text{doubly degenerate}) = K + {}^1/_2 V_{100}. \qquad (1)$$

The relative locations of E_F and K can be readily changed by varying the ratio c/a ($\partial(K/E_F)/\partial(c/a) > 0$). It is well known that when T = 0 zinc (c/a = 1.830[5]) has at the point K electronic "needles," i.e., $K_1 < E_F$, whereas cadmium (c/a = 1.863[6]) has no such needles, i.e., $K_1 > E_F$. In order to observe the passage of the level K_1 past E_F, the c/a parameter of zinc is increased by raising the temperature,[5] and that of cadmium is decreased by introducing a magnesium impurity.[7]

The single crystals needed for the investigation were prepared by zone growing (using equalization in the melts) from zinc and cadmium of purity not worse than 99.999% and magnesium of 99.99%.

METHOD AND RESULTS OF INVESTIGATIONS

As shown in the earlier investigations, the monotonic part of the magnetic susceptibility of non-transition me metals can serve as a very sensitive characteristic of the occupation of states separated by small energy gaps, with the peak of the diamagnetism revealing the instant of passage of the extremum of the band past the Fermi level.[8] The susceptibility was measured in the temperature interval 4.2–300°K in analogy with the preceding investigation.[9] Inasmuch as the peak of the diamagnetism on the temperature dependence of the susceptibility of zinc was observed and discussed earlier (see [8]), we only refined its position at H → 0 by measuring the anisotropy of the susceptibility with a torsion balance with self-compensation, the thermocouple being secured directly to the sample.

The main experimental results were as follows.

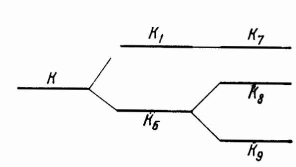

FIG. 1. Probable scheme of the splitting of the level K upon successive application of the lattice potential and the spin-orbit interaction (according to [4]).

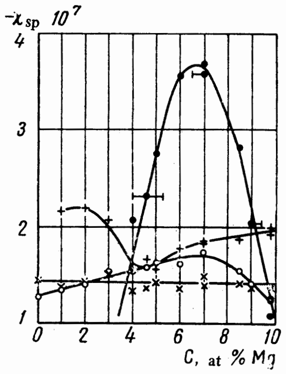

FIG. 2. Magnetic susceptibility of cadmium-magnesium alloys:

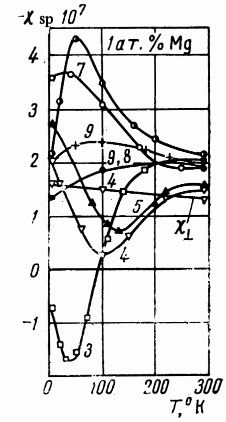

FIG. 3. Temperature dependences of the susceptibility of certain cadmium-magnesium alloys (the figures on the curves denote at.% of Mg).

1. The maximum of the diamagnetism on the temperature dependence of the susceptibility of the zinc is observed in the sixfold-axis direction ($\chi_{\parallel}$) at $T_0(H \to 0) = 112° \pm 0.5°K$.

2. The maximum of the diamagnetism on the concentration dependence of the susceptibility of the cadmium-magnesium alloys is observed on the same component at 6.5 at.% of magnesium and T = 4.2°K (Fig. 2).

3. With increasing temperature, the singularities of the concentration dependence of the susceptibility shift towards the larger magnesium concentrations, and their amplitude decreases (Figs. 2 and 3).

4. The alloy with 1 at.% magnesium reveals a distinct maximum in the temperature dependence of $\chi_{\parallel}$ (Fig. 3).

5. The temperature and the magnesium impurity have little effect on the second component of the susceptibility ($\chi_\perp$).

DISCUSSION OF THE RESULTS

The connection between the peak of the diamagnetism of zinc with the vanishing of the electronic needles, i.e., with the passage of the level K_1 past E_F with increasing c/a, follows from the direct experiment on the de Haas–van Alphen effect.[10] This means that

$$V_{100} = K - (E_F + kT_0), \qquad (2)$$

where in (1) we use in lieu of E_F the upper limit of the occupied states with allowance for the thermal excitation, inasmuch as the maximum diamagnetism is apparently reached when the states in the band under consideration are fully freed.[8] Assuming that the Fermi level corresponds to free electrons, and using for the calculation of K data on c/a at T_0 from [5], we get $V_{100} = -0.0063$ Ry. This value (taking into account the shift of the (100) plane) is in splendid agreement with the results obtained by Harrison[1] in the same approximation from the de Haas–van Alphen effect.

Indirect evidence confirms the analogous nature of the peak of the susceptibility of the cadmium alloys: it is observed on the same component (Item 2), i.e., the participating states are those at the vertical edges of the Brillouin zone with small masses in the basal plane, and for almost the same c/a ratio. Assuming that the temperature dependence of c/a of alloys does not depend on the composition, we get from [6,7] and from (1) that $V_{100} = -0.0065$ Ry.

It follows from Item 3 that the temperature dependence of the susceptibility is due essentially to variation of c/a, and not to the competing influence of the thermal excitation of the electrons; however, the role of the latter in cadmium is larger than in zinc, and therefore the peak under consideration does not appear in the temperature dependence. The cause of the increasing role of the thermal excitation in the susceptibility of cadmium may be the more compact arrangement of the levels. Indeed, the singularity of the behavior of $\chi_{\parallel}(T)$ of an alloy with a small magnesium content, noted in Item 4, predicts the existence of one more susceptibility peak near 0.5 at.%, i.e., at the point K there is one more level exceeding E_F by $\sim 5\times 10^{-4}$ Ry. This may be the level K_8, which is obtained from K_5 as a result of spin-orbit splitting (Fig. 1). It corresponds to the hole states, confirming the absence of a cavity inside the "monster";[11] its position determines the magnitude of the spin-orbit splitting $\Delta_K \approx 0.007$ Ry.

Details of the behavior of the susceptibility of weak solutions of magnesium in cadmium, and also of alloys with other components, are the subject of further research.

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