xperimental confirmation of the gap character of he electronic spectrum of disordered alloys in the egion of the structural instability

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We discuss the behavior of the magnetoresistance near the mobility thresholds. It is shown that when the Fermi level goes through the energy gap, the magnetoresistance reverses sign. Measurements were made of the magnetoresistance in the alloy system Ti_{1-x}–Cr_x; it is shown that the electron spectrum of this system has, in the region of the structural instability, a strong mobility singularity of the gap type. It is proposed that such a singularity is possessed by all binary alloys based on Ti with cubic transition metals. It is proposed to use the magnetoresistance to measure the gap parameter in those cases when this cannot be done by direct methods.

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It is known[1,2] that there exists a large group of binary systems, including alloys of Ti, Zr, and Hf with cubic transition metals, which is characterized by a number of general anomalies in the inetic and structural properties. The most pronounced singularities in the kinetic properties are he abrupt increase of the residual resistivity near a certain concentration x_{cr}, and the reversal of he sign of the temperature coefficient of the resistance on going through this concentration. According to structure data,[4] this concentration is favorable for the formation of the ω phase in he alloys.

Both anomalies were investigated in detail in a number of papers,[1–3] but their cause seems to emain unexplained to date. It was proposed in[5], on the basis of an analysis of the resistivity, the Hall coefficient, and the thermoelectric power of Ti_{1-x}–V_x alloys, that a gap may exist in the onduction-electron spectrum. This assumption makes it possible to explain from a unified point of iew the observed anomalies, including those indicated above. At the same time, the presence of uch a singularity in the electron-state density of a binary system whose initial components are metals cannot be obvious and must unconditionally be confirmed by experiment. This, however, aises considerable difficulties because of the small size of the gap. Estimates based on data on the onductivity yield for the gap a value of 10^{-2} eV. Thus, The suggested gap is almost unobservable y optical spectroscopy.

We show in this article that there is another possibility of confirming the appearance of a gap or of a deep pseudogap), by measuring the magnetoresistance, and we shall demonstrate the xistence of such a singularity in the density of states of the indicated alloys, using the Ti_{1-x}–Cr_x ystem as an example.

There is a general cause for magnetoresistance,[6] not connected with any concrete mechanism f conduction-electron scattering. The magnetic field either increases or decreases (depending on he spin direction) the Fermi energy by an amount $\pm\mu_B H$, where μ_B is the Bohr magneton. If the onduction of the electrons is determined by their end-point energy, then in the presence of a magnetic field the change of the conductivity takes the form

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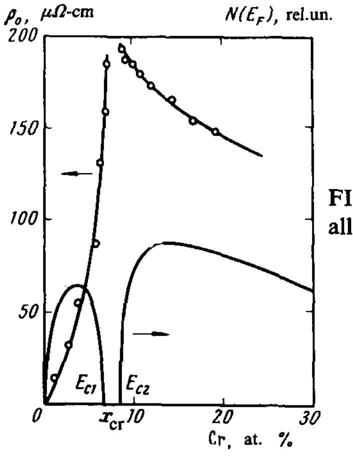

FIG. 1. Circles—behavior of residual resistivity of Ti_{1-x}–Cr alloys, solid—proposed behavior of the state density.

$$\delta\sigma = \tfrac{1}{2}\sigma''(E_F)(\mu_B H)^2, \qquad (1$$

where $\sigma''(E_F)$ is the second derivative of the conductivity with respect to energy, taken at the Fermi level. It is easily seen from this expression that: a) by virtue of the smallness of $(\mu_B H)^2$, the magnetoresistance effect can actually be observed only if the conductivity (density of states, carrier mobility) has a strong dependence on the position of the Fermi level (Fig. 1), b) the sign of the effect is determined by the position of the Fermi level relative to the corresponding singularity in the state density. The last circumstance is the most significant, since it is precisely the reversal of the sign of the magnetoresistance with increasing Fermi energy, from positive to negative, which signifies the existence of a gap (or a deep pseudogap) in the state density. It should be noted that a shallow minimum in the state density can lead only to a negative magnetoresistance, in as much as in this case $\sigma''(E_F) > 0$.

Thus, if we are able to vary the position of the Fermi level with the aid of an external parameter, say the density, then near x_{cr} (Fig. 1) we can hope to observe the magnetoresistance connected with expression (1). The effect will then be positive at $E_F \approx E_{c1}$ and negative at $E_F \approx E_{c2}$. The magnitude of the effect should decrease rapidly with increasing distance from x_{cr} in either direction (Fig. 1).

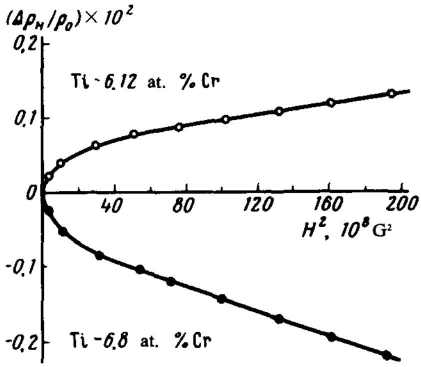

FIG. 2.

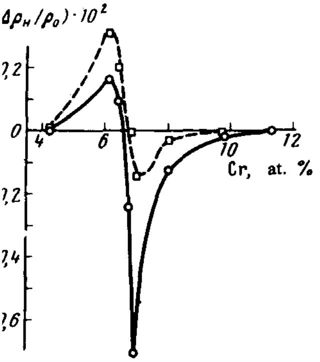

FIG. 3. Squares—magnetoresistance in a field of 150 kOe at $T=4.2$ K. Circles—the same at $T=20.4$ K.

To verify experimentally the foregoing possibility we measured the magnetoresistance of the lloys Ti_{1-x}–Cr_x ($x=4.3$, 6.12, 6.4, 7, 8, 9.8, and 11.3 at.%) in fields up to 200 kOe and at emperatures $T=4.2$ and 20.4 K. Figure 2 shows the results of measurements for two samples, ith 6.12 and 6.8 at.% Cr. As expected, the samples were divided into two groups, depending on he sign of the effect. As to the sign of the effect, for the experimentally observed resistivity change $\rho_H/\rho_0 \sim 0.2\%$ in a field $H=2\times10^5$ G and at $\rho_0=200$ μΩ cm, the conductivity at $E_F=E_{c1}$ (or E_{c2} should change by an approximate factor of 10^3. Such a change corresponds, both in order of agnitude and in its meaning, to the mobility jump discussed in[6].

The concentration dependence of the magnetoresistance in a field $H=150$ kOe at $T=4.2$ and 0.4 K is shown in Fig. 3. This dependence was obtained for alloys for the first time ever, and can pparently serve not only as a qualitative but also as a quantitative characteristic of the gap. In this ase it is natural to take the gap parameter to be the distance between the extrema of the curve of ig. 3. As seen from the figure, these extrema are sufficiently well prononced, so that it is possible o measure the width of the gap with good accuracy. From the data on the K-emission spectra[7] we an determine the value of dE_F/dx. For the Ti_{1-x}–Cr_x system this value is 0.016 eV/at.%. The gap arameter determined from Fig. 3 is then 0.014 eV, in good agreement with the value obtained rom data on the electric conductivity assuming semiconductor conduction.

Thus, the results can be regarded as an experimental confirmation of the assumption made n[5] concerning the character of the electron spectrum in alloys based on titanium, and the ollowing conclusions can be drawn: 1) A strong singularity of the gap type or of the mobility gap ype appears in the electron spectrum of the considered binary systems, particularly in the i_{1-x}–Cr_x system; this singularity manifests itself in a distinct behavior of the concentration ependence of the magnetoresistance (Fig. 3). 2) The magnetoresistance can be used as a tool to etermine the gap parameter in those cases when this is difficult to do by direct methods; the easurement accuracy is limited only by the accuracy with which the sample composition and E_F/dx are determined.

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