METAL–INSULATOR TRANSITION IN MOTT–HUBBARD SYSTEM FeSi*

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Following to the comprehensive study of a steady magnetic field dc- and ac-transport and magnetization in the almost magnetic narrow-gap semiconductor FeSi the galvanomagnetic measurements have been carried out in pulsed magnetic fields up to 50T. It was shown from the analysis of the experimental data obtained on high quality single crystals of iron monosilicide that the Mott–Hubbard scenario of metal–insulator transition with on-site Coulomb interaction $U \approx 3$D (D-is the band half-width) provides the most adequate description of the low temperature anomalies in this model system. From this point of view the pulsed field magnetoresistance and Hall coefficient anomalies may be also interpreted in terms of a MIT in a strong magnetic field.

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During the last decade the almost magnetic narrow-gap semiconductor iron monosilicide was usually classified as Kondo-insulator [1] and additionally FeSi was presented as the model material to study the hopping conductivity, Anderson localization and this type metal–insulator transition (MIT) [2, 3]. From this point of view FeSi at low temperatures ($T < 100$K)

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needs to be described in term of insulator and a various kind substitution of Si (to Al, Ge *etc.*) was applied to induce the transition from insulator to metal [2, 3].

On the other hand recent comprehensive studies of a steady magnetic field dc- and ac-transport [4], thermopower [5] and magnetization [6] in combination with the results of microwave and optical measurements [7, 8] of FeSi allowed to conclude in favor of the Mott–Hubbard scenario of MIT with on-site Coulomb interaction $U \approx 3D$ [9] (D is the band half-width). In the framework of the developed approach the Hubbard-type correlations-spin fluctuations between the e_g and t_{2g} type states of Fe were deduced as the most important factor which is dominant in physics of this strongly correlated electron system.

In particular, from the high precision magnetization data it was established in [4, 6] that the low temperature phase of FeSi may be described adequately as a strongly correlated metal (SCM) with a magnetic moment of charge carriers $\mu_{\text{eff}} \approx \mu_{\text{B}}$ (Fig. 1, μ_{B} — Bohr magneton). Moreover, very strong renormalization of the density of states (DOS) at E_{F} occurs resulting to a dramatic increase of the paramagnetic response below liquid nitrogen temperature (Fig. 1). The Pauli-like paramagnetic contribution appears to be very sensitive to the magnetic field and it decreases drastically (by a factor of $3 \div 4$) in moderate fields $\mu_0 H \leq 12$T [6].

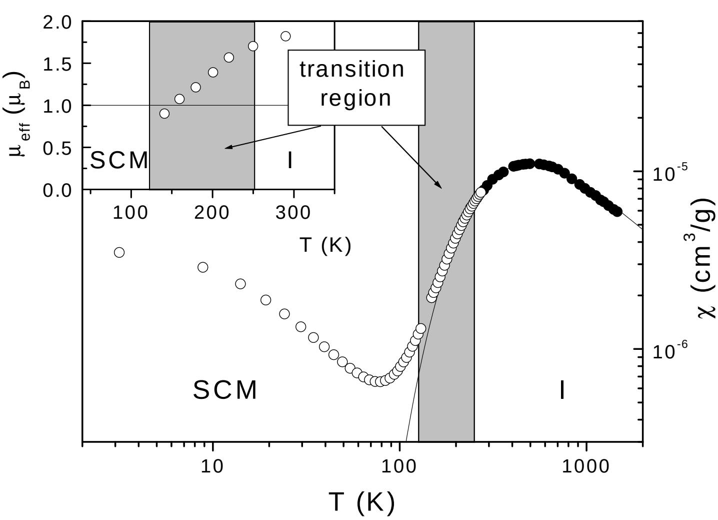

Fig. 1. Magnetic susceptibility of FeSi in a wide temperature range. Inset shows the temperature dependence of the effective magnetic moment μ_{eff} of charge carriers. The Mott–Hubbard type MIT range is also shown (I — insulator, SCM — strongly correlated metal).

As a result the Mott–Hubbard transition in FeSi is arranged as *insulator-to-metal transition* from high temperature phase of FeSi which can be identified as **a narrow-gap semiconductor** (I in Fig. 1, the gap between e_g and t_{2g} Hubbard bands $\Delta_g = U-2D \approx 60$ meV [4–6]) to **a very narrow-band metal** (SCM in Fig. 1, a width of the spin-polaron resonance of DOS at E_{F} is $E_p \approx 6$ meV [4–6]). Thus, this picture is just opposite to that one proposed in [1–3] and it provides one with the most adequate description of the low temperature anomalies in this model system.

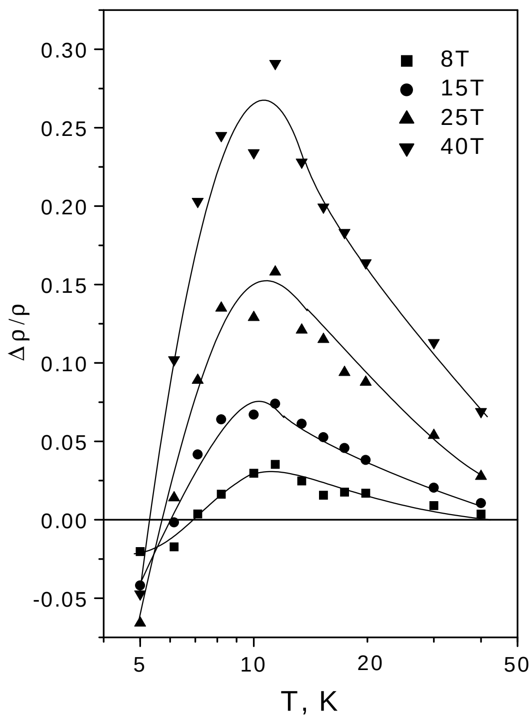

Fig. 2. Magnetoresistance of FeSi in steady (8T) and pulsed magnetic fields.

Additionally, to involve more arguments in the discussion of the nature of MIT in FeSi in the present investigation pulsed field galvanomagnetic measurements have been carried out in magnetic fields up to 50 T. It is worth to mention that the effect of strong magnetic field is very different for Kondo-insulator and for strongly correlated Mott–Hubbard metal. Indeed, in the first case negative magnetoresistance should be dominant as a sequence of a depression of Kondo-compensation mechanism in high magnetic field. The effect of magnetic field on Mott–Hubbard system has been studied theoretically in [10] where it was shown that large positive magnetiresistance needs to be expected for strongly correlated metal. The data of Fig. 2 are in good agreement with the prediction of [10] and it contributes certainly in favor of the proposed scenario of the Mott–Hubbard type MIT. At the same time the amplitude of the positive magnetoresistance component (Fig. 2) is too large to be attributed to the simple kinetic contribution $\Delta\rho/\rho\sim H^2$ because of a small enough values of the charge carriers' mobility $\mu_{\rm H}<10$ cm^2/Vsec in FeSi [11].

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