Large Coulomb gap in the spectrum of localized states of Mn in amorphous Si

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A Coulomb gap Δ has been detected in the energy spectrum of the localized states of Mn in amorphous Si near the metal-insulator transition. This gap was determined from the temperature dependence of the conductivity within the context of a theory developed by Shklovskiĭ and Éfros. The value of Δ was found to be more than an order of magnitude larger than the values found previously for semiconductor-impurity systems with shallow levels.

Coulomb interaction of an electron and a hole, trapped at the centers between which there is a transfer of charge carriers, leads to a change in the spectrum of the states near the Fermi level with the appearance of the Coulomb gap: a region with a sharply reduced state density[1] which appears in experiments on low-temperature conductivity. It is difficult to identify the Coulomb gap in amorphous semiconductors because the resistance of samples becomes large (10^{12}–10^{15} Ω·cm) as the temperature is lowered, making it impossible to carry out measurements. The temperature at which the Coulomb gap can first be seen in the conductivity, according to Refs. 1 and 2, is given by

$$T^{+} \cong e^{6} g / k^{2} \kappa^{3} T_{1}, \tag{1}$$

where e is the electronic charge, g is the density of localized states, k is Boltzmann's constant, κ is the dielectric constant, and T_1 is a constant which depends on the

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ties of the material. It follows that the density of localized states must be increased in order to raise T^+ on condition that the system remains on the insulator side of a metal-insulator transition.

A more striking manifestation of the Coulomb corrections may be seen in an amorphous Si (a-Si), in which there is an impurity with deep levels, since the wave function of an electron is strongly localized in this case. As a result, a large density ($\sim 10^{21}$ cm^{-3}·eV^{-1}) of localized states can be reached before the system undergoes a transition to the semimetallic state, which occurs according to Mott's criterion,[3] at $g^{1/3}\, a \sim 0.25$ (where a is the localization length). An increase in the density of localized states decreases the length of the jump and hence increases the Coulomb interaction between the carriers.

In this letter we identify the correlation effects in experiments on low-temperature conductivity of a-Si doped with Mn, whose solubility in the lattice structure of Si is considerably higher than in a crystal. This higher solubility accounts for the high values of the impurity states with deep levels in the material studied.

The samples were obtained by the method of electron-beam evaporation of silicon in a vacuum and then introducing manganese into silicon by ion implantation. To achieve uniform distribution of Mn in the film, we have varied the ion energy between 50 and 230 keV. During irradiation, the temperature was held near room temperature.

As the impurity concentration was increased from 10^{19} to 5×10^{21} cm^{-3}, the conductivity of the a-Si:Mn samples increased from 10^{-5} to 60 $(\Omega\cdot\text{cm})^{-1}$. Analysis of the temperature dependence of the conductivity $\sigma(T)$ over the temperature interval $500 > T > 4$ K (Fig. 1) showed that at low temperatures $80 > T > 4$ K, the functional

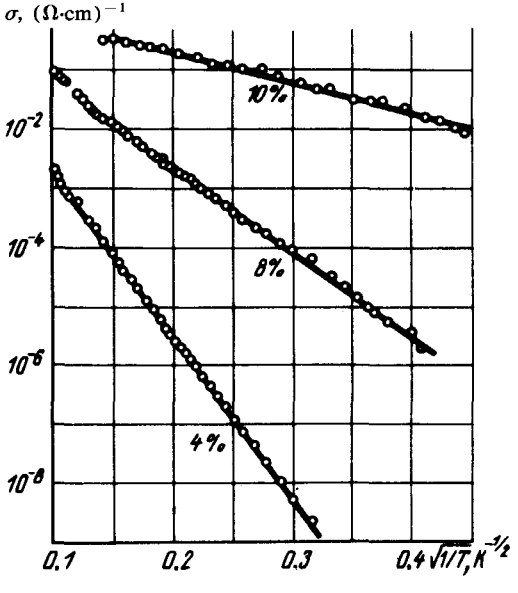

FIG. 1. $T^{-1/2}$ dependence of the conductivity of a-Si:Mn samples with various impurity concentrations.

TABLE I.

Sample	N cm^{-3}	N at. %	T^+ K	T_1 K	Δ meV
1	2×10^{21}	4	80	4290	25
2	4×10^{21}	8	50	1040	10
3	5×10^{21}	10	35	130	3

dependence $\sigma(T)$ of the samples with the impurity concentrations 2×10^{21}, 4×10^{21}, and 5×10^{21} cm^{-3} varies as

$$\sigma=\sigma_0 \exp\left[-(T_1/T)^{1/2}\right],\ T_1=\beta e^2/k\kappa a\,, \tag{2}$$

where β is a constant (according to Ref. 4, $\beta\cong2.8$).

A functional dependence of this sort can be interpreted in terms of a parabolic Coulomb gap in the localized-state spectrum.[1] The gap width Δ can be determined from the relation[2,5] $\Delta=(K/2)\times(T_1T^+)^{1/2}$. In Table I we present the values of T_1, T^+, and Δ which turned out to be an order of magnitude larger than analogous values for semiconductors (including[6] a-Si) doped with shallow-level impurities. As the concentration of the impurity is raised, the gap shrinks and at $N>12$ at.% the gap disappears because of the transition of the system to a semimetallic state. After such a transition, the temperature dependence of the conductivity acquires, as we know, a power-law form: $\sigma(T)=\sigma_0+\sigma_0T^n$, where $0<n<1$. For a-Si:Mn samples containing

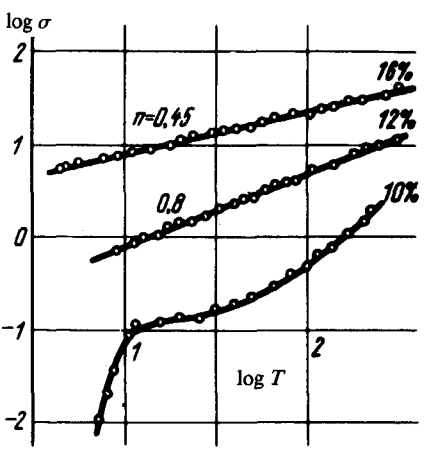

FIG. 2. Temperature dependence of the conductivity of a-Si:Mn samples near the metal-insulator transition.

12 and 16 at. % of the impurity, the $\sigma(T)$ curves acquire a linear form in $\log \sigma$ and $\log T$ coordinates (Fig. 2). The values of n are 0.8 and 0.45, respectively, for the concentrations indicated above.

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