Surface States in a HgTe Quantum Well and Scattering by Surface Roughness


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Scattering of two-dimensional electrons in wide ($d = 18–22$ nm) HgTe-based quantum wells has been thoroughly studied. The mobility has been found to reach a maximum and then to decrease at two-dimensional electron densities above $(2–6) \times 10^{11} \text{cm}^{-2}$ owing to scattering by roughness of the quantum well. The theory of scattering by roughness has been elaborated taking into account transformation of the wavefunction with an increase in the electron density. Good agreement of this theory with the experiment indicates the existence of surface states at the interfaces of the wide HgTe quantum well.

HgTe quantum wells are currently among the most intensively studied objects of physics of two-dimensional electron systems (2DESs). This is primarily associated with a unique gapless energy spectrum of a 2DES in a HgTe quantum well, which is largely determined by relativistic effects and, consequently, by the spin–orbit interaction. Equally important is the fact that very high-quality HgTe quantum wells can be grown owing to recent progress in molecular-beam epitaxy of II–VI compounds. As a result, several new kinds of low-dimensional electron systems, namely, two-dimensional topological insulators, a two-dimensional semimetal, and two-dimensional gapless Dirac fermions, have been implemented in these quantum wells in the last years [1–6].

As is known [7], the scattering of electrons by surface roughness is the leading scattering mechanism in inversion surface layers at a high carrier density because the layer thickness decreases and the transverse quantized electron momentum increases with an increase in the field pressing the electrons. As will be seen below, the experimental dependence of the mobility in a HgTe layer also agrees with this picture. However, in the case of a HgTe quantum well, the localization of the wavefunction inside the quantum well varies depending on the magnitude of the electron wave vector $k$ in the quantum well. At $k < \pi/d$ (where $d$ is the well width), the maximum electron wavefunction square is situated in the center. However, at $k > \pi/d$, it splits into two. The formed maxima shift toward the well boundaries with an increase in $k$ (each maximum shifts toward a certain boundary; the direction of the shift depends on the direction of electron motion along the boundary), ultimately forming surface states at the well boundaries. Such behavior of the electron wavefunction was predicted in [8] and confirmed by more accurate calculations in [9]. Experimental indication of the existence of such states is of undoubted interest.

In this work, we perform theoretical and experimental investigation of electron scattering by roughness at the interfaces of wide HgTe quantum wells, the width of which is a few times greater than the critical one ($d_c = 6.3$ nm) corresponding to the transition from the direct to inverted spectrum. We show that the scattering of two-dimensional electrons by well roughness starts to dominate at densities $N > 3 \times 10^{11} \text{cm}^{-2}$. We elaborate the theory of 2D electron scattering by this roughness taking into account transformation of the wavefunction with an increase in the electron density predicted in [8, 9]. Comparative analysis of the theory and experiment indicates the emergence of surface states at the interfaces of wide HgTe quantum wells with an inverted spectrum.

We start with the description of the experimental and experimental results. The samples under investigation were 50-μm-wide field-effect Hall structures made of undoped 18–22-nm HgTe quantum wells with the (013) and (100) orientations and a distance of 100 and 250 μm between potentiometric contacts (see inset in Fig. 1). The fabrication technology was described in detail in [10]. The measurements were carried out at a temperature of 4.2 K in magnetic fields up to 1 T with the use of a standard lock-in detection at a frequency of 12 Hz and an excitation current through the sample of 100 nA, which excludes heating effects. The depen-
Differences of the dissipative ($\rho_{xx}$) and Hall ($\rho_{xy}$) components of the resistivity tensor of the samples under investigation on the gate voltage $V_g$ are shown in Fig. 1. The shown curves are typical of 18–22 nm quantum wells, in which a two-dimensional metal–two-dimensional semimetal transition occurs under a change in the gate voltage \[3, 10, 11\]. The $\rho_{xx}(V_g)$ curve has a maximum situated near the charge neutrality point, whereas $\rho_{xy}(V_g)$ changes its sign to the left of the charge neutrality point. In this work, we will be interested only in the gate voltages at which the quantum wells of interest contain a two-dimensional metal with a parabolic spectrum. This corresponds to the electron densities $N_s > 5 \times 10^{10}$ cm$^{-2}$ \[3, 10\] and $N_s > 1 \times 10^{10}$ cm$^{-2}$ \[11\] for the (013) and (100) orientations, respectively. The experimental density dependences $\mu(N_s)$ of the electron mobility for several samples are shown in Fig. 2 (the basic characteristics of these samples are given in Table 1). As is clearly seen, the behavior of all $\mu(N_s)$ curves is qualitatively the same: the mobility increases at low $N_s$ values, reaches a maximum of $(4–7) \times 10^5$ cm$^2$/V s, and then starts to decrease. A more detailed comparison shows that the region of increase, as well as the positions of the maximum and the beginning of a decrease in the mobility, can vary depending on the sample. In particular, the position of the maximum is $N_s \approx 2 \times 10^{11}$ cm$^{-2}$ for samples 100623_1 and 110615 and $N_s \approx 6 \times 10^{11}$ cm$^{-2}$ for samples 110614 and 081112. The above behavior of the two-dimensional electron mobility at liquid helium temperature takes place in many 2DEs, from the inversion channels of silicon MOS transistors \[7\] to 2DEs in AlGaAs/GaAs heterojunctions \[12\]. In all cases, it indicates two scattering mechanisms: by impurities, which dominate at low $N_s$ values, and by roughness, which prevails at high $N_s$ values. However, while scattering by impurities can be described with the use of the already known relations (see, e.g., \[13\]), the problem of scattering by roughness cannot be considered within the standard approach \[7, 12\], in which the localization of the wavefunction changes owing to a considerable change in the shape of the quantum well. First, the shape of the well remains almost unchanged at the gate voltages used in this experiment owing to a high well depth (about 0.5 eV). Second (and most important), as was mentioned above, there is a much stronger effect in wide quantum wells associated with the emergence of surface states at the interfaces of the wide HgTe quantum well with the inverted spectrum. Thus, scattering by roughness in such a well requires separate consideration with allowance for the transformation of the wavefunction in the well. Below, we describe the theory developed for this case. It is assumed that the states $\psi$ of electrons and holes in the quantizing HgTe layer can be found with the use of the Luttinger Hamiltonian \[8\] with zero boundary condition $\psi = 0$ at the $z = \pm d/2$ interfaces of the HgTe layer and the basis $\phi_{\alpha}^{(j)}(k, q)\exp(ikr + iqz)$ of solutions in

**Table 1.** Basic characteristics of the samples under investigation

<table>
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<th>Sample</th>
<th>Orientation</th>
<th>$d$, nm</th>
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