Dipole trap model for the metallic state in gated silicon-inversion layers

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In order to investigate the metallic state in high-mobility Si-MOS structures, we have further developed and precised the dipole trap model which was originally proposed by B. L. Altshuler and D. L. Maslov [Phys. Rev. Lett. 82, 145 (1999)]. Our additional numerical treatment enables us to drop several approximations and to introduce a limited spatial depth of the trap states inside the oxide as well as to include a distribution of trap energies. It turns out that a pronounced metallic state can be caused by such trap states at appropriate energies whose behavior is in good agreement with experimental observations.

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I. INTRODUCTION

The discovery of the metal-insulator transition (MIT) in two-dimensional (2D) electron systems in 1994[1,2] has attracted large attention, as it was in apparent contradiction to the scaling theory of localization[3,4] which states that in the limit of zero temperature, a metallic state should exist only in three dimensional systems, whereas in two dimensions disorder should always be strong enough to induce an insulating state. The MIT in high-mobility n-type silicon inversion layers shows a strong decrease of resistivity ρ towards low temperature T for high electron densities, manifesting the metallic region, whereas a strong exponential increase of ρ demonstrated the insulting regime for low densities. A similar but weaker behavior was observed in many other semiconductor systems at low densities and low temperatures (e. g. p-GaAs,[5] n-GaAs,[6] SiGe,[7] AlAs[8])

Several models were suggested in order to explain the unexpected finding of metallic behavior in 2D. The most important ones are i) temperature-dependent screening,[9–14] ii) quantum corrections in the diffusive regime,[15–18] and iii) quantum corrections in the ballistic regime.[19,20] Numerous argumentations for the different models are given in literature,[21–25] but a clear decision for one of them could not been drawn yet.

As an alternative, Altshuler and Maslov (AM) introduced the dipol scattering scenario for Si-MOS structures in which charged trap states in the oxide layer form dipols together with the image charge of the screening 2D electrons.[26] The interplay between the gate voltage dependent energetic position of the trap states and the height of the chemical potential may lead as well to a metal-insulator transition in that system. It should not be assumed that the dipol scattering effect is active alone, as the temperature dependence of screening and quantum corrections will surely contribute at low temperatures, but the charging of trap states might be the generator of the particularly large effect in Si-MOS structures. It is known that the misfit at the silicon/silicon-oxide interface produces charged defect states in the thermally grown oxide layer.[27–29] Arguments on the importance of trap states in Si-MOS structures were also given by Klapwijk and Das Sarma.[30]

AM could show within their analytical calculations that a trap level at energy E_T which is either filled or empty, depending on its position relative to the Fermi energy E_F, can lead to a critical behavior in electron scattering if E_T and E_F are degenerate. This dipole trap model is able to explain the main properties of the metal-insulator transition in gated Si-MOS structures.

For the analytical calculations AM made a number of assumptions. These are:

a1) the trap states possess a δ-like distribution in energy (i. e. have all the same energy),

a2) the spatial density distribution in the oxide is homogeneous,

a3) the states occupied with electrons behave neutral and cause no scattering of 2D electrons whereas the unoccupied states are positively charged and lead to scattering (AM work in the hole trap picture, but we describe occupation in terms of electrons),

a4) a charged trap state is screened by the 2D electrons so that the resulting electrostatic potential can be described by the trap charge and an apparent mirror charge with opposite sign on the other side of the interface,

a5) the scattering efficiency of the 2D electrons is described by a dipole field of the trap charge and its mirror charge,

a6) a parabolic saddle-point approximation for the effective potential between the Si/SiO2 interface and the metallic gate was used in order to perform analytical calculations,

a7) the energy of the trap state E_T is fixed relative to the quantization energy E_0 of the 2D ground state inside the inversion potential, and

a8) the chemical potential μ in the 2D layer has (A) either the same temperature dependence as in the bulk