

If the dimensions of the electronic conductor are small enough, the conduction electrons pass through the conductor without any collisions with the vibrating crystal lattice and also without any electron-electron collisions. Due to the absence of these (inelastic) collisions, the conduction electrons behave like waves and their wave properties affect directly the macroscopic electrical properties of the conductor, for instance its electrical conductance. Such conductor is called mesoscopic, because its electronic properties are somewhere between “micro” and “macro”, namely, they are determined by the wave mechanics known from the microscopic world of atoms, although the conductor is still composed of a large (macroscopic) number of atoms.

Of particular interest is the mesoscopic ring - a small ring-shaped conductor. If the opening of such ring is penetrated by constant magnetic flux, the ring supports the persistent electron current that circulates around the ring in principle forever. This current exists despite the absence of any voltage source and flows without any Joule heat dissipation. The aim of our research is to describe the mesoscopic conductors from the first physical principles. We have already developed the first-principles quantum transport simulation of the conductance/current in a mesoscopic conductor/ring with realistic disorder due to the polycrystalline grains, impurity atoms, and rough sample edges. We also study the electron conductance and persistent current in a mesoscopic ring which is pierced by external magnetic flux and in the same time connected to two mesoscopic leads biased by external voltage. This situation is a nano-electronics analog of the Aharonov-Bohm effect known from the elementary quantum mechanics. In particular, we are interested in the effect of the strong magnetic field which produces the edge electron states known from the quantum Hall effect. Moreover, we are interested in the effect of self-induction when the persistent current is solely due to the magnetic field generated by the persistent current itself and no external flux is needed. We hope that our theory will show the self-induced regime for several hundreds of vertically-stacked mesoscopic rings. Our mesoscopic studies can help to understand what happens when the microelectronic devices are reduced towards the mesoscopic dimensions.

Of great practical importance are the transport properties of the nano-crystalline metal-oxide semiconductors like  $\text{TiO}_2$ ,  $\text{SnO}_2$ ,  $\text{HfO}_2$ ,  $\text{Ta}_2\text{O}_5$ , and other similar metal oxides. For instance,  $\text{TiO}_2$  already reached a commercial success as a sensor of dangerous gases (like hydrogen) and nowadays it is a candidate for a new type of the non-volatile memory, the so-called resistive-switching memory. We investigate theoretically the physics beyond these two applications.

Concerning the gas sensor, the present research is focused mainly on the development of the highly-sensitive  $\text{TiO}_2$  gas sensors that work at room temperature and are compatible with planar semiconductor technology. We study the electron transport in a layered Pt –  $\text{TiO}_2$  - Pt nano-sandwich that consists of a thin (~ 30 nm) nano-crystalline  $\text{TiO}_2$  layer embedded between the bottom Pt electrode (the supporting layer below the  $\text{TiO}_2$  layer) and top Pt electrode on the

top TiO<sub>2</sub> surface, shaped as a narrow stripe of width  $w$  as small as 80 nm. The typical size of the TiO<sub>2</sub> grains is  $\sim 10$  nm and they are normally the semiconductors of  $n$  type. However, the conduction electrons escape from the grains on the top of the grain surface where they are bound by the excess oxygen molecules. As a result, the TiO<sub>2</sub> layer is highly resistive. The hydrogen molecules, if any, penetrate into the TiO<sub>2</sub> layer via the inter-grain diffusion and after some time react with the bound electron-oxygen complexes. This reaction gives rise to the water molecules (they diffuse out of the TiO<sub>2</sub> layer) and to the free conduction electrons. As a result, the device resistance decreases and this decrease can be quite pronounced, depending on the amount of the hydrogen and geometry of the sensor. In particular, experiments of our colleagues from the Comenius University show that if the sensor with  $w$  below  $\sim 100$  nm is subjected to the air with 1 % of H<sub>2</sub>, its resistance response,  $R_{\text{air}}/R_{\text{air+H}_2}$ , is as large as  $10^7$  and the response time is as short as a few seconds even at the room temperature. We want to explain theoretically the mentioned experiments. Moreover, we want to design theoretically an ideal Pt – TiO<sub>2</sub> – Pt sensor. In both cases the resistance of the Pt – TiO<sub>2</sub> - Pt nano-sandwich has to be calculated in the atmosphere without hydrogen and with hydrogen, and the calculation has to include the electric fields as large as  $\sim 4 \times 10^5$  V/cm. Due to the high electric fields one has to deal with the hot electron transport. Moreover, one has to consider the spatially dependent resistivity of the TiO<sub>2</sub> layer, caused by the exponentially decaying diffusion profile of hydrogen below the top Pt electrode.

The non-volatile TiO<sub>2</sub> memory based on the resistive switching resembles the sensor structure discussed above, however, the thickness of the TiO<sub>2</sub> layer is now as small as the grain size ( $\sim 10$  nm) and the TiO<sub>2</sub> layer is intentionally grown as oxygen deficient. The pure TiO<sub>2</sub> is a large gap semiconductor. However, in the oxygen deficient TiO<sub>2</sub> layer there is a significant concentration of the oxygen vacancies and these vacancies behave like shallow donors. In such case the TiO<sub>2</sub> layer behaves like an  $n$  type semiconductor and the resulting layer resistance between the Pt electrodes is strongly dependent on the actual spatial distribution of the donors. If one applies a strong enough electric field, one can vary the spatial distribution of the donors from a highly-resistive distribution to the low-resistive one and vice versa. This happens at fields  $\sim 10^6 - 10^7$  V/cm, which are one order of magnitude stronger than the fields in the gas sensor. The ionic motion responsible for the resistive switching is usually described by a standard drift-diffusion theory, in which the ions are thermally accelerated by the Joule heating of the crystal lattice. However, such theory fails to explain some anomalous features of the measured resistive switching times, namely a sudden six orders of magnitude decrease of the forming time at a certain critical field. We want to develop the theory capable to explain the mentioned anomalous feature. We work beyond the standard drift diffusion theory by considering microscopically a coupled hot electron hot ion transport .