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QUANTUM PROCESSES IN SEMICONDUCTING MATERIALS AND SPINELECTRONICS

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Abstract. A short overview is given of recent advances in the field of nano semiconductors, which are suitable as materials for spin polarized transport of charge carriers. On the basis of last theoretical and experimental achievements, it is shown that development of diluted and wide forbidden zone semiconductors with controlled disorders as well as their molecular structures is the very prospective way for magnetic semiconductors preparation and quantum computing systems.

1. INTRODUCTION: CONTROLLED DISORDERS, NANOSCIENCE, NANOTECHNOLOGY AND SPINELECTRONICS

Nanostructures constructed from inorganic solids like semiconductors have new electronic and optical properties considerably different from that of the common crystalline state due to their size and quantization effects [1,2]. The quantization effects reflect the fundamental characteristics of structures as soon as their size falls below a certain limit. An example of the simplest nanostructure is the quantum dot formed from the energy well of certain semiconductor materials with 5-10 nm thickness sandwiched between other semiconductors with normal properties.

Quantum dots, for example, have lead to important novel technology for lasers, optical sensors and other electronic devices. The application of nanolayers to data storage, switching, lighting and other devices, can lead to substantially new hardware, for example energy cells, and eventually to the quantum based internet.

Nanoscience and nanotechnology encompasses the development of nano spinelectronics, spinelectronics materials production, nano spinelectronic measuring devices and technologies. Nano spinelectronics, based on usage of magnetic semiconductors, represents new area of science and engineering. The reason to that is the perspective of development and creation of principally new materials and devices for information technologies operating as charge, and spin degree of freedom of carriers, free from limitations inherent for metal spinelectronic devices. The main structural property of materials in which we can observe novel nano dimension phenomenas is their unperfection – high concentration of different defects connected with several impurities of metal a non-metal chemical elements. So, novel very exiting properties of semiconductors are determined by impurities and their disordered distribution. At the same time the last theoretical and experimental achievements have shown that disorders in semiconductors should be controlled – should have a necessary rules and regulations.

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2. FEATURES OF TRAVELLING ELECTRICAL DOMAINS ON LOCALISED STATES

It was shown [3] that current oscillations in the circuit observed in weakly compensated semiconductors in the hopping conductivity region are associated with "hopping" domain periodic formation and travelling in the bulk of the sample; the domain motion probably occurs along dead end sections of the hopping network, responsible for the drooping region in the current-voltage characteristic [4]. It is also shown [5] that hopping domains is of triangle shape with equal leading and back edges. The dependence of the shape of current oscillations observed in the hopping conductivity region in a weakly compensated p-Si on the supply voltage applied to the sample is established. With increasing bias voltage the current pulse shape to form a hopping domain changes significantly. The change in the shape is ascribed to voltage redistribution in corresponding regions in the bulk of the crystal.

The phenomenon manifested itself in a periodic current increase and decrease observed in the external electric circuit. The current oscillations were observed in samples with a sub linear current-voltage characteristic in the portion with a negative differential resistance. Fig. 1 shows the dependence of the current density j of sample p-Si with boron impurity concentration Na = $5{,}9\cdot10^{16}$ cm^{-3} and compensation degree $K = 4\cdot10^{-5}$ on electric field E at T = 10K. As soon as the j-E characteristics begins to flatten out one observes an onset of current oscillation, which suggest a region of negative differential conductivity.

In general terms, the phenomenon is in accord with notions of electrons trapping network of acceptors, which governs the ohmic hopping transport. As it is known the ohmic hopping transport is governed by the infinite cluster of acceptors, whose separation does not exceed $r_c+a/2$, where $r_c = 0.87N^{-1/3}$ is the percolation radius. The extraction of the infinite cluster is shown in Fig. 2. The characteristic length of the infinite cluster network is $L = 1/3\ (r_c/a)^{\nu}Na^{-1/3}$, where $\nu = 0.88$ is a critical index [6]. Typical dead ends of the infinite cluster are of the same order. At weak electric field when $eEL << kT$, an electron can easily hop in and out of such dead ends. But at strong electric field when $eEL >> kT$, the probability to escape from a dead end oriented against field is reduced by a factor exp(-eEL/kT).

If the escape out of such dead end along the electric field can occur only by hop with the length highly exceeding r_c then that dead end is a trap for an electron. Thus with the ever-growing electric field a great fraction of electrons is found in traps. As a result the conductivity decreasesexponentially with the increase in E:

$$\sigma(E) = \sigma_0 \exp\left(-\frac{eEL}{2kT}\right), \qquad (1)$$

Eq. (1) leads to a negative differential resistance when $E > 2kT/eL$.

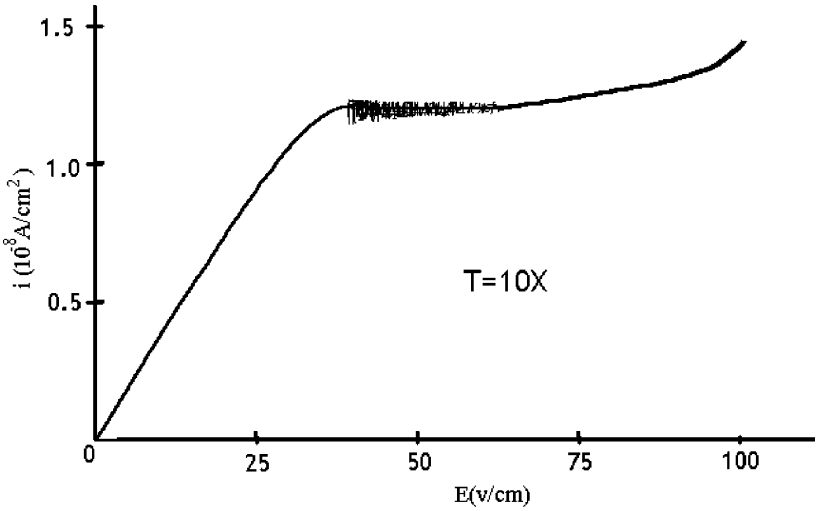

Fig. 1. Behavior of the current density as E increases slowly with time (the total duration of the sweep is 10 min.

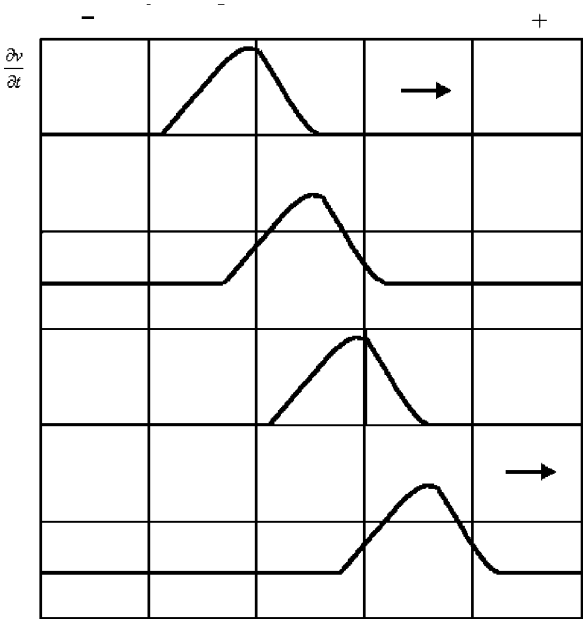

Fig. 2. Dependence of *dV/dt* on the distance *x* at different *t*. The time period between curves is 25 ms. Scale of abscissa: one point = 0.125 cm.

In order to reveal the nature of domain instability, we studied potential varying distribution along the sample surface, using the capacitor probe. The time evolution of *t* was observed directly on the oscilloscope connected to the capacitor probe through a high impedance prod and electrometric amplifier (no lateral coordinate dependence has been detected). Samples investigated have resistance of the order of 10^9 Ω and very small operating currents (10^{-9} A) thus a protective electrode screen was used in the cable connector. The protective screen was connected to the follower with small output impedance, which allowed excluding effectively capacitive and resistive leakage currents since potential difference between signal wire and its environment was equal to zero. A sensing element of the probe was made of a metallic foil strip with the protective electrode and external earthen screen in the form of two strips on one side of it; those strips were separated by the thinnest strip of plastic material. On the other side of foil the probe's sensing element was separated from the sample also by a sheet of plastic. In measurements of domain parameters a specially made gold needle was also used as a potential probe sliding along the sample surface.

If we consider the dependence of *dV/dt* on *X* at various *t*, as shown in Fig. 3 for arbitrarily chosen *t* values, we can see a well formed maximum of 150 mm in width, which moves to the anode with the velocity approximately equal to 0.25 cm s^{-1} . The average field within can be estimated by the maximum width and voltage drop. It is about 300 V/cm.

Fig. 3 shows the *E*(*x*) profiles of uniformly travelling stable domains formed after application of different voltages from the voltage generator to the sample p-Si with boron impurity concentration *Na* = $7.3 \cdot 10^{16}$ cm^{-3} and compensation degree *K* = $2 \cdot 10^{-4}$. The curve (a) corresponds to the voltage V_{th} = 56 V or to the strength E_{th}= 86 V/cm. The curve (b) was obtained in the trigger regime with V_{tr} = 51 V corresponding to E_{tr} = 78 V/cm. In this case the domain was formed by a short pulse V_{form} = 58 V > V_{th} with duration $t = 3 \cdot 10^{-2}$ s. From the diagrams it is clear that the domain is of triangle shape at these voltages with equal leading and back edges. The leading edge of the domain is depleted with hopping electrons; its positive charge is formed by the uncompensated charge of the ionized donors. The back edge is enriched with slow hopping electrons accumulated due to a decrease in their velocity at the cluster dead ends with increasing field.

As we noted the generation took place at a certain critical bias voltage U_t. A voltage generator was

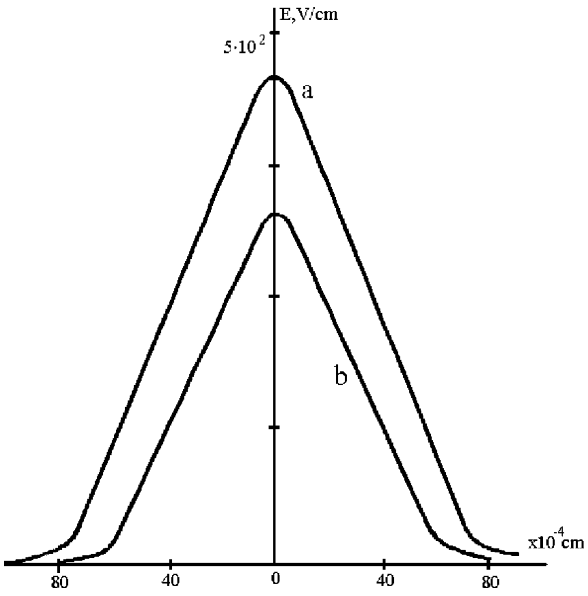

Fig. 3. The *E*(*x*) profiles of uniformly traveling stable domains formed after the application of different voltages (curve a corresponds to the field strength E_{th} = 86 V cm^{-1}; curve b was obtained in the trigger regime with E_{tr} = 78 V).

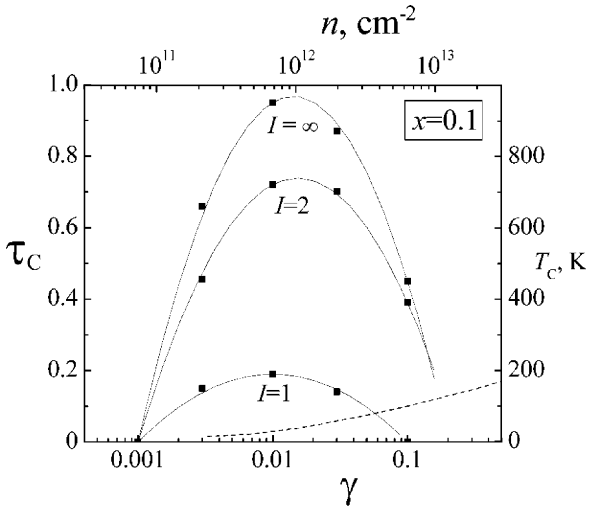

Fig. 4. Dependencies of Curie temperature on the carrier concentration for the system with the concentration of magnetic impurities x=0.1 for various interaction strengths I. The dashed line is corresponding to I≈1.

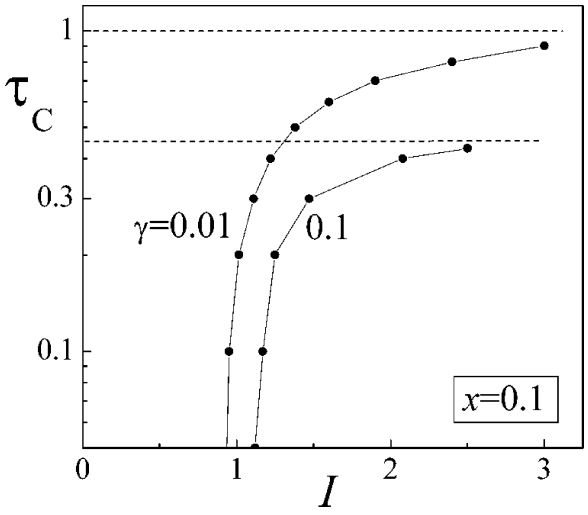

Fig. 5. Dependencies $\tau_C(I)$ of Curie temperature for two-dimensional system with the concentration of magnetic impurities x=0.1 at various carrier concentrations determined by the parameter γ.

switched to the sample in the pulse mode. The voltage pulse width could be controlled in the broad range. The current meter was a specially designed differential amplifier. Part of the signal was applied to the protective screen of triaxial cable from the amplifier output due to the feedback. Here capacitance leakages were neutralized thus increasing the frequency properties of the current meter. The form of the varying current signal was observed on the oscillograph and recorded on the photographic film. The process of domain formation depends on many conditions. In particular, on the type of contacts and on the conditions imposed by the external circuit.

Let us consider the change in the current pulse shape in the sample with Na=7.3·10^{16} cm^{-3} and K≈2·10^{-4} at the bias voltage Us close to the threshold of high field region formation. In this case the pulse width was 3-4 of the transit time T. The investigations were carried out at temperature 10K. In Fig. 5, b, c, and d, a time dependence of the current shape is given for three fixed bias voltages within 38.4-41 V. In this region the time-averaged current increases with increasing voltage. Here, on the cathode there occurs a triangle-shaped domain moving towards the anode. The formation of the next domain is preceded by a certain expectation time decreasing with the bias increase. At the bias voltage equal to the domain formation threshold, the differential mobility $\mu_d=dv/dE$=0 (here v is the carrier drift velocity); so, in our case, the Kroemer criterion is fulfilled [7].

Therefore when the bias field even slightly exceeds the threshold one, i.e. at a low$|\mu_d|$, the domain can be formed. And the higher is $|\mu_d|$, the quicker it is formed. At weak circuit screening, the domain was formed due to various kind of interference; in this case, the pulse repetition period depended on the pulse value and the accidental character of interference occurrence.

It is clear that the time dependence of the current reproduces the conductivity profile in a certain scale in the region of in homogeneities. With increasing bias the domain velocity does not change significantly. One should also take into account that the observed in homogeneity (the relief of the lower part of the current pulse) in the sample is due to a monotonous rise in the conductivity in the portion of approaching the anode. Therefore with increasing bias a stronger domain passes a longer distance to the anode. Knowing its velocity V_c ≈ 0.25 cm^{-3} and the size d ≈150 mm, a characteristic time of its travel to the anode can be estimated τ_a≈ 60 ms. It should be mentioned that this process is actually much more complex. For example, the action of the Poole-Frenkel hopping effect accompanying the domain motion should probably be taken into account [8].

With a further increase in the bias voltage in the sample, a new domain may appear on the cathode simultaneously with the motion of the domain to the anode. Here the constant voltage applied to the sample is redistributed between the domain moving towards the anode and the domains being formed. At the same time the maximum value of the generating current remains unchanged.

During the motion of the high field region towards the anode, the voltage excess on the cathode increases for the time longer than that of a space charge formation. Therefore this voltage will form one domain in the sample. Here, taking into consideration the tendency in development of the current pulse shape, one can assume that at a high bias voltage the domain becomes wider and takes a trapezoidal shape. In our case the complex relief of the current pulse can be explained by inhomogeneities in the short path of the domain as well as by the mutual effect of the domain moving to the anode and those being formed.

Voltage pulses with the width equal to the domain transit time were also applied to the sample. The front pulse rise of the bias voltage took place for the time much shorter that the Maxwell time $\tau_{md}=\varepsilon/4\pi q\mu_d n_0$ of formation of a volume charge (where ε is the substance permittivity, q is the charge, μ_d is the differential mobility, n_0 is the carrier concentration). In this case, the current pulse shape observed was different from that of current oscillations taken at a constant voltage source. Therefore, at the sample voltage close to the threshold of formation of current oscillations, there occurs a situation when the first domain is formed. In this case, conditions are created for main diode transit regimes – the quenching regime and the lagging regime similar to the transit regime of a Gunn diode. With sufficiently high bias voltage, the conditions of voltage redistribution between the domain moving towards the anode and the next domain being formed on the cathode are realized. The formation of adjustable in homogeneities in the sample makes it possible to control the current with time, which presents a practical interest in terms of creation of analog devices working at low temperatures.

3. QUASI-TWO DIMENSIONAL DILUTED MAGNETIC SEMICONDUCTORS

Diluted magnetic semiconductors, such as $Ga_{1-x}Mn_xAs$ are broadly investigated in connection with their potential for new electronics developments and, especially, spin electronics. For explanation of the ferromagnetism in those compounds the known RKKY-mechanism of the indirect exchange interaction is recruited [9,10] which leads to the correct estimating the Curie temperature in the framework of the traditional mean field theory (MFT). Mn-atoms (with concentration Nm) substituting for Ga-atoms introduce in the system the own magnetic moments and, in addition, as acceptors deliver free holes (with concentration n). It is precisely those holes become to be carriers responsible for the interaction. However, the equality of the concentrations $n=N\mu$ keeps only at low Mn-concentrations ($x \le 0.05$), so that the carrier concentration is usually less than the concentration of magnetic impurities: $n=\gamma N\mu$ where the coefficient of the impurity "efficiency" $\gamma<1$. Nevertheless, the concentration of magnetic impurities, delivering carriers, in actual systems is usually so high that the impurity band is formed which at $x \ge 0.01$ merges into the valence band. Even though, the carrier concentration occurs to be not so high that one could consider them as highly degenerated ones within the whole (being of interest) range of relatively high temperatures. Furthermore, it is important that the carrier concentration is almost independent of the temperature: $n=\gamma N\mu\approx$Const.

Although two-dimensional structures represent the most natural systems for the embedding in the traditional semiconductor technology, almost all theoretical works are dealt with the threedimensional systems of degenerate carriers. Similarly, most of experimentally studied systems are threedimensional ones. Magnetic features of two-dimensional semiconductor systems with magnetic impurities interacting by RKKY-mechanism via carriers of arbitrary degeneracy has been recently considered in the paper [11] where it has been shown that reducing the system dimension (from 3D to 2D) results in the significant lowering of the Curie temperature.

Using the generalized mean field theory [12] for systems with the indirect interaction of magnetic impurities and taking into account the randomness of their spatial arrangement, by Ising approximation and supposing that the indirect coupling between magnetic moments of impurity atoms is realized by means of RKKY interaction upon system properties are described with the help of the distribution function of local values of the field arising as a result of magnetic ions' coupling with their own

surroundings. In real systems, the scattering of those fields proves to be very substantial.

The expression has been derived for the energy $w(r)$ of indirect RKKY interaction for two parallel spins $\boldsymbol{S}_1$, $\boldsymbol{S}_2$ of magnetic ions spaced at the distance r in the two-dimensional system with degenerated carriers:

$$w(r) = -\frac{m}{4\pi h^2}\left(\frac{J_{ex}}{N}\right)^2 F(r) S_1 S_2,$$
$$F(r) = -\int_0^{k_F} k N_0(kr) J_0(kr) dk, \qquad (2)$$

where J_{ex} is the exchange energy for interaction of a spin with a free charge carrier of the mass m, N is the concentration of lattice atoms ($N=1/a^2$ for the square lattice of the period a); J_0, N_0 are Bessel functions. The result generalized to the case of the arbitrary degeneracy (with the Fermi energy ε_F of any value) reads

$$F(r,T) = -\frac{1}{r^2}\int_0^{\infty} \frac{y N_0(y) J_0(y) dy}{1+\exp\left[\dfrac{\hbar^2 y^2}{2mr^2 - \varepsilon_F} / k_B T\right]}. \qquad (3)$$

Behavior of the function (3) is determined not only by the temperature but also by the temperature dependence of the Fermi energy.

In the framework of the standard two-dimensional band and under the invariable carrier concentration, the ratio $\eta=\varepsilon_F/k_B T$ is defined by the relation

$$e^{\eta(T)} = e^{\frac{\pi h^2 n}{m k_B T}} - 1, \qquad (4)$$

that predicts negative hvalues at T=100K if $n \le 10^{12}$ cm^{-2}. Taking into account Eq. (4), the expression (2) could be written in the form $w(\rho) = -J_{eff}\phi(\rho,\tau)\boldsymbol{S}_1\boldsymbol{S}_2$, where $J_{eff}=(ma^2/4\rho h^2)J_{ex}^2$,

$$\phi(\rho,\tau) = -\frac{1}{\rho^2}\left[e^{\frac{2\pi^2\gamma\alpha}{\tau}} - 1\right]\int_0^{\infty} \frac{y N_0(y) J_0(y) dy}{e^{\frac{2\pi^2\gamma\alpha}{\tau}} + e^{\frac{y^2}{\rho^2\tau}} - 1} \qquad (5)$$

$\rho=r/a$ is the reduced separation between interacting impurities, $\tau=2\pi m a^2 k_B T/\eta^2$ is the reduced temperature (for GaMnAs $\tau \approx 10^{-3} T$ [K]), $x=N\mu/N$ is the relative concentration of magnetic impurities. In the most actual case of the intermediate degeneracy, the function (5) has been estimated by numerical calculations.

Let the system consisting of randomly arranged and oriented Ising spins be in the state characterized by the average reduced magnetization $0 \le j \le 1$. The total interaction energy $W=S_i w_i$ of a given spin $\boldsymbol{S}_1$ with other spins $\boldsymbol{S}i$ (i=2,3,…) is a random value which we shall define by the effective local magnetic field $H=-W/\mu$ ($\mu=g\mu_B[S(S+1)]1/2$) and describe by the distribution function $F(j;H)$ depending on the average concentration Nm of effective magnetic ions and the reduced system magnetization $j=2\chi-1$ where χ is the average fraction of spins of "magnetoactive" ions directed "up". Farther calculations very well described in [13] have shown that prepared final equation predicts the phase diagram of the system, temperature dependencies of its magnetization (in ferromagnetic phase) and susceptibility (in paramagnetic phase), as well as the dependence of Curie temperature on the interaction strength, the relative magnetic ion concentration $x=N\mu/N$ and the relative free carrier concentration $\gamma=n/N\mu$.

This equation has the solution corresponding to the ferromagnetic state ($j>0$) under the condition

$$\frac{H_j}{\sigma} > \sqrt{\frac{\pi}{2}} \qquad (6)$$

that means that the effective RKKY-field proportional to H_j has to "overpower" not only the thermal disordering but also the scattering of local fields proportional to σ. The upper boundary τ_C^{max} of the temperature range where the cited condition is satisfied determines the maximum attainable temperature of the ferromagnetic ordering at infinite interaction energy ($I \to \infty$).

Curie temperature at the finite interaction energy could be determined by solving the equation. Relevant non-monotone dependencies $\tau_C(\gamma)$ are displayed in Fig. 4. To compare, the dashed line in Fig. 4 reproduces the dependence $\tau_C(n)$ obtained in the framework of the standard MFT. The optimal carrier concentration occurs to be on the order of 10^{12} cm^{-2}, that is significantly lower than the predicted value $n \sim 10^{14}$ cm^{-2}.

In addition, Fig. 5 demonstrates a threshold value of the interaction strength I to drive the system in the ferromagnetic state. This is to be contrasted with the result of the standard mean-field theory that predicts no such a threshold.

4. SPIN – POLARIZED TRANSPORT IN SEMICONDUCTORS

The essential effort of the scientists is concentrated on studying of the spin-polarized transport in nanosize multilayer structures, which are including alternating layers of ferromagnetic metals and non-magnetic semiconductors. Operation of a spintronic device requires efficient spin injection into a semiconductor, spin manipulation, control and transport, and spin detection. The relevant role in solution of this problem is shunted to search and investigations of new ferromagnetic materials, which are capable to be reliable and good spin injectors. The magnetic discrete alloys are very promising among such objects. They are multilayer systems composed of submonolayers of a ferromagnetic material in the matrix of a non-magnetic semiconductor, for example, Mn/GaAs or Mn/GaSb. It is well known, that these alloys have high Curie temperatures and sufficiently high spin polarization. The circumstance is not less important that it is possible to control and to manage of the "ferromagnetic metal - semiconductor" boundary surface immediately during the synthesis of these materials.

As it was investigated recently, they should be prepared only by the methods of the MOS hydride epitaxy and laser epitaxy with usage of pulsed annealing of epitaxial layers. Perspectives of development and creation of new types of a non-volatile memory stipulate the significance of spintronics with random access (MRAM), quantum single-electron logical structures, and ultra dense information storage media. Thus, elementary information storage unit will be represented by an electron spin. The realization of the spin-polarized current transfer opens out new possibilities for the solid-state electronics also. For instance, there are observations of the spinpolarized luminescence and creation of the high frequency diodes, output characteristics which ones one can change by an external magnetic field. Another example is the possibility of creation of a new generation of narrowband devices of the solid-state electronics of millimetre and submillimeter wave ranges like generators, amplifiers, receivers and filters, modulated and frequency tuned by magnetic field and fully current controlled [14].

The discovery of giant magnetoresistance effect (GMR) can be considered as new important step for development of spintronics. This phenomenon is observed during the study of thin films with alternating layers of ferromagnetic and non-magnetic metals. It is found that, depending on the width of a non-magnetic spacer, there can be a ferromagnetic or antiferromagnetic interaction between magnetic layers, and antiferromagnetic state of magnetic layer can be transformed in ferromagnetic state by an external magnetic field. The spin-dependent scattering of conduction electrons is minimal, causing a small resistance of material, when magnetic moments are aligned in parallel, whereas for antiparallel orientation of magnetic moments the situation is inversed. The effect GMR brightly has demonstrated, that a spin-polarized electrons can carry magnetic moment through non-magnetic materials.

Namely the GMR effect was used in a new generation of the magnetic field sensors, which appeared in 1994 as commercial products on market The implantation of this technology has allowed more than on the order to increase a density of the information storage on magnetic disks. The sensors operating with the tunnel magnetic junctions (MTJ) fall into the second class spintronics devices. Very thin dielectric layer divides their ferromagnetic electrodes, and electrons are tunnelling through a nonconducting barrier under influence of applied voltage. The tunnel conductivity depends on relative orientation of the electrode magnetizations, and tunnel magnetoresistance (TMR) it is small for parallel alignment of magnetizations of electrodes and is high in opposite case. New memory devices include storage units based on the MTJ structures and allow not only to increase essentially the storage density and the access speed to a memory, but also to provide complete saving of data at disconnecting of a power supply. A disadvantage of these devices is the small scale of integration, bound with necessity of usage of additional controlling transistors. Possibility to overcome these limitations is connected nowadays only with the development of the semiconducting spintronics, and, in particular, with the creation of spin transistors. In this case spintronic devices cannot only switch or to detect electrical and optical signals, but also to enhance them, and also to be used as multifunction units. Due to this reason, the third direction of development spintronic devices is based on the development of multilayer nano structures of ferromagnetic semiconductors, which demonstrate properties not available for their metal analogs. There is possibility to control by electric field a magnetic state of material and the giant planar Hall effect, which exceeds on several orders of magnitude the Hall effect in metal ferromagnets.

The super-giant TMR effect observed for the first time in epitaxial MnAs (or MnSb) as well in manganese containing layers. The discrete alloys have high Curie temperatures (above 300K for the GaSb-system), demonstrate extraordinary Hall effect at high temperatures, and have a relatively high degree of the spin polarization. It is possible in such systems to control not only quality of the border "ferromagnetic metal – non-magnetic semiconductor", but also manage of the current carrier's concentration and change the type of magnetic ordering. The discrete alloys should be considered as random magnet systems owing to hardly inhomogeneous allocation of a magnetic phase in submonolayers.

The interest in so called diluted magnetic semiconductors is given an impetus by the recent demonstration of the ferromagnetic critical temperature T_c =110K in GaMnAs. To date, most theoretical models proposed assume that the holes occupy a Fermi sea in the valence band [13].

Theoretical models of the virtual crystal approximation have been used to study the influence of disorder on transport and magnetic properties of magnetic semiconductors. The Boltzmann equation with Born approximation scattering rates has provides estimates of Anizotropic Magneto resistance Effect of order up to 12%. The key of understanding the kinetic and magnetic anisotropy effects is a strong spin-orbit coupling in the basic semiconductor valence band.

The most striking feature in off-diagonal conductivity coefficients for example in (GaMn)As and other arsenide and antimonide of diluted magnetic semiconductors occurs is the large anomalous Hall effect, which occurs because of spin-orbit interactions. In the metals standard assumption is the Anomalous Hall arises because of spin-orbit coupling component in the interaction between band quasiparticles and crystal defects, which can (Ga,Mn)As/GaAs/(Ga,Mn)As structures is not less promising for applications.

So-called magnetic discrete alloys to days are of the most prospective materials for solution of the spin injection problem. These alloys involve a periodic system of sub-monolayers of magnetic ions (for example, Mn), placed between semiconducting layers (GaAs, GaSb, InAs) forming a magnetic superlattice. There are as incidentally distributed Mn ions and 2D magnetic islands of lead to skew scattering with Hall resistivity contribution proportional to diagonal resistivity. For diluted magnetic semiconductors the Anomalous Hall effect is based on spin-orbit coupling in the Hamiltonian of the ideal crystal and implies a final Hall conductivity even without disorder. The Hall fluid effective Hamiltonian theory discussed without free parameters and it is reliably in materials with high critical temperatures where halls are metallic.

The effects of the $As_{Ga} – As_i – V_{Ga}$ transition to the ferromagnetism of (GaMn)As can be explained by the Mulliken orbital populations of the *d*-shell for both majority and minority spins and the corresponding spin polarization for the ferromagnetic configuration. In this case the ferromagnetic coupling is strengthening considerably by the distortion, and that all together the energy splitting and Mulliken orbital population of Asi VGa are the very similar to those of defect free (GaMn)As. These suggest that the ferromagnetic order in (GaMn)As is unaffected by the presence of Asi VGa pairs. This result is in agreement with the hole-mediated picture of ferromagnetism, and can understood by noting that Asi VGa defects energy levels show minimal splitting in (GaMn)As [15].

More detailed studies of disorders will combine Kondo description of the spin interactions as well as relevant Monte Carlo techniques applied to both metallic and insulating conditions.

5. MODELING OF QUANTUM SYSTEMS THE WAY OF QUANTUM DEVICES DESIGN

Development of novel nanotechnology based informatics determines of necessity of instruments, which able to manipulate with elementary particles localized in Angstrem (0.1 nm) size. The main way of the building of that size particle based structures is so called self assembling, which should be controlled by outside influence directly and indirectly. The simulation and modeling of self assembling processes nowadays is only instrument, which can rightly oriented the very quick substructural (time o nuclear configuration change approximately compares 1 nanosec) processes towards preparation of ordered substances and materials. Usage of special computing programs is helping to energy clusters (e.g. molecules) preparation, which can working as photon energy collectors as well as energy accumulators for the nano robots and nano computers.

Quantum system simulation and modeling works are elaborating atom and molecular scale physical effects which give the possibility to open the novel approaches for the superconductivity,

superfluidity, and other very important phenomena. In all above mentioned works the main problem is quantum computations, which is still most complicate and less exact. Quantum simulation is based on two rules among which the first is very sufficient: Dynamical trajectories of the *n* quantum systems are always sustainable; and the second very complex: For the system of *n* simple quantum particles (quantum bits – qubits) number of degree of freedom increase as 2^n, which means that in time of addition of any particle complexity increases two times. For example for modeling of hydrogen molecule sintesis, where four particles are participating (twenty cubits each) it is necessary to have a memory 1024, which is more then worldwide computers memory today. The popular and successful route for the solving of this problem even for the case of systems of hundreds of electrons is the suitable approximation in the model building processes.

Generally, following R. Feinman's idea it seems possible in the future to build self developed computing device, and, at the same time create the new software, which permitting to elaborate models at the quantum level.

There are several positive results in the way of quantum computers creation: Nuclear Magnetic Resonance approach for liquid substances reaches up to 10 qubits, Josephson transitions method for solids – 2 qubits [16]. Following that for the hydrogen task accomplishment it is necessary to use 80 logical qubits. For the moment it is very difficult within real experiments to build quantum system based working computing device. At the same time so called virtual experiments and simulations are well developed. Using Hartree-Fok, diffusion, density function and other methods the relevant computing programmes were elaborated [17]. These programmes, the final part of which often is the visual models, present the crucial points for structural calculation in modern physics and chemistry. It necessary to underline that dynamics of quantum conditions for its right observation needs drawing of elementary particles of electromagnetic field (photons), and in addition the mechanisms of quantum electrodynamics [18]. Last achievements have shown that quantum systems simulation and modeling is possible to organize by using the existing computers. By the several groups of scientists the relevant computing programmes were elaborated and at the first stage the real models of simple quantum systems were developed [19].

Quantum calculations as well as quantum conditions simulation are the key point for investigation of atomic and molecular processes in different substances and nanoscience and nanotechnology development.

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