Dependence of the magnetic properties of MnGaN epitaxial layers on external electrical field

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Abstract: Investigation of the magnetic properties of MnGaN epitaxial layers as a function of external electrical field was performed on the basis of field effect structure. The structure included substrate of n-type GaN, epitaxial layer of n-type Mn$_x$Ga$_{1-x}$N, dielectric layer and metal layer acting as field effect device gate. Each Mn atom in Mn$_x$Ga$_{1-x}$N contributes 4 net spins due to the electrons occupying energy levels $^4$F, $^4$D, $^4$P and $^4$G belonging to 3d orbital, and these levels are in the energy band gap and in the top of the valence band of Mn$_x$Ga$_{1-x}$N. The position of the Fermi level is determined to be in the energy band gap of the layer of GaN and to be above the level $^4$F in the layer of Mn$_x$Ga$_{1-x}$N. In this way application of external negative voltage on the gate causes change in the number of electrons contributing net spins and the saturation magnetization $M_{sat}$ of Mn$_x$Ga$_{1-x}$N changes as well. It was found that $M_{sat}$ changes in the range $1.15 \times 10^{-3}$ to $0.7 \times 10^{-3}$ Aµm$^{-1}$ if the external voltage changes in the interval 0 -- 5V. The application of this structure for the design of spintronic devices is discussed in this paper.

Keywords: Nitride Semiconductors • Spintronics • Field Effect Device

1. Introduction

The author’s recent results [1] in theoretical investigation of the magnetic properties of Mn$_x$Ga$_{1-x}$N were confirmed experimentally [2,3] by independent research. These results are connected with the spin of the electrons belonging to 3d orbital of the Mn atom, which can be considered to be a precondition for magnetic properties of Mn$_x$Ga$_{1-x}$N. It is expected that these properties would have a possible application in spintronics and hence it determines the scientific efforts for investigation of the impact of Mn atom, which substitutes on Ga site in the structure of Mn$_x$Ga$_{1-x}$N [4–8]. A Field effect device based on change of the magnetic properties of layers of Mn$_x$Ga$_{1-x}$N due to application of external voltage is the subject of consideration in this paper. The device contains sandwich layer structure: substrate of n-type GaN – epitaxial layer of n-type Mn$_x$Ga$_{1-x}$N (active layer) – dielectric layer – metal layer (acting as field effect gate). The author’s results [1] that give the electron band structure of Mn$_x$Ga$_{1-x}$N and the positions of $^4$F, $^4$D, $^4$P and $^4$G energy levels of electrons belonging to 3d orbital of Mn atom are used. The position of the Fermi level in the energy band diagram of the field effect device was determined. The saturation magnetization $M_{sat}$ of Mn$_x$Ga$_{1-x}$N layer was found to be a function of the voltage applied on the gate of the device, and the change of $M_{sat}$ with variation of the gate voltage was determined. The application of this device in spintronics is discussed.

2. Experimental Procedures

Cross-sectional area of the field effect device is provided in Fig. 1. It contains n-type GaN substrate as the basis. The purpose of this layer is to provide electrical connection to the bottom of Mn$_x$Ga$_{1-x}$N layer and to be technological substrate for the deposition of the next layer. The layer of Mn$_x$Ga$_{1-x}$N is called the active layer, and the magnetic properties of this layer are subject of
change. Each Mn atom in Mn$_x$Ga$_{1-x}$N contributes 4 net spins due to the electrons occupying energy levels $^2F$, $^4D$, $^6P$ and $^8G$ belonging to 3d orbital of this atom. The purpose of the dielectric layer is to provide electrical insulation between the metal layer and the active layer. It can be SiO$_2$. The thickness of this layer is important and it must be as thin as possible in order for the low gate voltage to be able to rule the magnetic properties of the active layer. The purpose of the metal layer is to act as a gate in the field effect device.

LCAO (Linear Combination of Atomic Orbitals) electron band structure (Fig. 2) of wurtzite Mn$_x$Ga$_{1-x}$N for points $\Gamma$ is calculated by previously developed method [9,10] and in consideration of the following conditions: a) Mn atom substitutes for a Ga atom saving the tetrahedral symmetry of the crystal cell; b) two of the valence electrons of isolated Mn atom occupy 4s orbital and other 5 valence electrons occupy $^4S$ level of the 3d orbital (according to Hund’s rule the electron spin of the ground state $^6S$ is 5/2); c) the Mn-N bond is ion-covalent and it has tetrahedral symmetry. Detail description of the calculation of the LCAO electron band structure is given in [1].
The occupancy of these levels depends also on the position of the Fermi level in conformity with the authors [2,3]. The comparison of both the theoretical results having place in this paper and the experimental data [2,3] shows a quality conformation of the theory.

2.1. Saturation magnetization of the active layer

Saturation magnetization is sum of all possible net spins aligning parallel to each other. Each Mn atom in the structure of MnGa_{1-x}N can contribute up to 4 net spins due to electrons occupying states 4G, 4P, 4D and 4F. (It is important to be noted that the total spin per atom Mn in MnGa_{1-x}N is 3/2 and it determines occupancies of states 4G, 4P, 4D and 4F, however the corresponding levels belong to the energy bands of MnGa_{1-x}N and therefore there are no orbital contributions to the magnetic moment per atom, i.e. only electron spins have to be accounted.)

The saturation magnetization $M_{sat}$ of certain region of the layer Mn_{x}Ga_{1-x}N is

$$M_{sat} = \sum_n \alpha \mu_p$$

(1)

Where the sum is over all Mn atoms in the region ($n$ is the number of the Mn atoms), $\alpha$ is integer number giving the electrons per Mn atom providing net spins ($0 \leq \alpha \leq 4$ and it depends on the occupancies of the levels 4G, 4P, 4D and 4F), and $\mu_p = 9.27 \times 10^{-24}$ A m$^2$ is Bohr magneton.

The occupancies of the levels 4G, 4P, 4D and 4F depend on the position of Fermi level $E_F$ and $M_{sat}$ for the region of Mn_{x}Ga_{1-x}N, which is under the gate, becomes

$$M_{sat} = \mu_p N W_\alpha L_\alpha \sum x \int (1 + \exp[(\xi(x) - E_F)/kT])^{-1} dx$$

(2)

Where $N$ is concentration of Mn atoms in the region, $W_\alpha$ and $L_\alpha$ are gate-width and gate-length respectively, $k$ is Boltzmann constant, and $T$ is temperature. The sum is over all 4G, 4P, 4D and 4F states designated as $\xi(x)$, and the integration is over the entire width $W'$ of the region (in fact $W'$ is the width of the layer of MnGa_{1-x}N). The quantity $\xi(x)$ is function of the coordinate $x$ having normal direction to the surface of MnGa_{1-x}N ($\xi(x)$ is function due to influences of electrical charges in the dielectric layer, the difference in the work functions of the gate-metal and of the MnGa_{1-x}N layer, and the gate-voltage $V_G$). It is found

$$\xi(x) = [(V_0+V_G)/W_0]^2 - 2[(V_0+V_G)/W_0] x + 4\xi_0 + V_0 + V_G$$

(3)

Where $V_0$ is potential due to both the influences of electrical charges in the dielectric layer and the difference in the work functions of the gate-metal and of the MnGa_{1-x}N layer, $W_0$ is width of depletion region in MnGa_{1-x}N due to the influences of both $V_0$ and $V_G$, and $\xi_0$ is equal to the energies of 4G, or of 4P, or of 4D, or of 4F respectively, which are provided in Fig. 2.

3. Results and discussion

The electron occupancy of the levels 4G, 4P, 4D and 4F is important regarding the quantity $M_{sat}$. Therefore the position of the Fermi level has to be established close to one of them and to be in conformity with the polarity of the gate voltage. There are several options but the impact of the occupancy of level 4D or that of 4F on $M_{sat}$ could be expected to be much more significant in comparison with the impacts of the occupancies of levels 4G and 4P, because the last two levels belong to the valence band of MnGa_{1-x}N. The option giving the impact of the occupancy of level 4F on $M_{sat}$ is chosen in this paper and it is considered the value of Fermi level $E_F = -4.65$ eV. It determines the position of $E_F$ above the level 4F and above the middle of the energy band gap of GaN (however $E_F$ remains in the energy band gap). This position of $E_F$ can be achieved by proper donor doping, which is possible to be performed technologically.

It is found that $W_0$ must be equal to $W'$ in order high sensitivity of $M_{sat}$ to be achieved. (In order this condition to be satisfied super-lattice MnGa_{1-x}N-GaN can be used instead of layer MnGa_{1-x}N if it is necessary due to technological reasons.) It is chosen $W_0 = W' = 4$ μm, and it is considered $V_G = 0.33$ V. Also it is chosen $W_0 = 20$ μm and $L_\alpha = 20$ μm. The dimensions $W'$, $W_0$ and $L_\alpha$ can be different however the volume of the active region is
related to the value of $M_{\text{sat}}$. Application of negative gate voltage is considered.

Calculations were performed according to (2) and (3), and the results are provided in Fig. 3 where $M_{\text{sat}}$ is presented as function of both $V_G$ (having variation in range $0 - -5V$) and $N$ (having variation in range $0 - 2.41 \times 10^{28} \text{ m}^{-3}$). The graphic shows that the higher sensitivity of $M_{\text{sat}}$ occurs for relatively high concentrations of Mn atoms in Mn$_x$Ga$_{1-x}$N and $M_{\text{sat}}$ changes in range $1.15 \times 10^{-3} - 0.7 \times 10^{-3} \text{ A \mu m}^{-1}$.

4. Conclusion

The results presented in this paper show that the magnetic properties of the semiconductor compound alloy Mn$_x$Ga$_{1-x}$N can be ruled by applied low voltage. This conclusion is important in terms of further technological development of field effect devices with application in spintronics. Also, the results show a possibility for the design of hybrid spintronic – optoelectronic devices based on both magnetic and optical properties of Mn$_x$Ga$_{1-x}$N.

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