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Temperature stable positive magnetic susceptibility of semiconductor wobbled nano rings

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Abstract. We theoretically investigate the magnetic response of ensembles of semiconductor nano rings. Using our mapping method we simulated geometrical and material dispersion of the magnetic susceptibility of ensembles of the rings. Unlike the susceptibility of an individual ring the averaged susceptibility shows small temperature effect.

1. Introduction

Recent experimental studies on self-assembled *InAs/GaAs* quantum nano-scale rings (NRs) demonstrate controllable flexibility of geometrical and material characteristics of those semiconductor nano-objects [1,2]. Three-dimensional topological quantum effects (similar to the Aharonov-Bohm effect) for electrons confined in a NR result in unusual behavior of the differential magnetic susceptibility (DMS) of the ring containing only a single electron [1,2,3]. The appearance of the positive peak in the DMS at low temperatures has to be addressed to the Aharonov-Bohm crossing between two lowest energy states of the electron confined in the ring. The actual experimental height of the peak and its temperature dependence were found in contradiction to the theoretical description performed in [1,2]. Unlike in the theoretical simulation results the experimental peak demonstrated a negligible temperature effect. It was proposed in [1] that the temperature stability is due to the rings' ensemble averaging, but no further theoretical or experimental considerations have been done to proof this point. At the same time the inherent property of the contemporary semiconductor self-assembled nano-objects is their geometrical and material parameters' dispersions. The general approach to the description of ensembles of semiconductor nano-objects is to consider a multi-parameter distribution (multi-dimensional) function including dispersions of all appropriate parameters' within wide ranges of their changes. This requires for a computational method which can optimize those extensive simulations of ensembles of semiconductor nano objects. Our mapping method (proposed in [4]) allows us to efficiently simulate quantum mechanical properties of semiconductor nano systems such as NRs. In this study using the method we address the issue of the temperature dependence of the magnetic response of ensembles of three-dimensional torus-shaped wobbled NRs.

2. Theoretical method and simulation results

To determine the magnetization M (total magnetic moment) and differential magnetic susceptibility χ for an isolated nano ring, the standard approach is to calculate the total electronic energy of the ring in the presence of the external magnetic field **B**. The magnetization and DMS of the ring are [3]

$$M = \sum_n \left(-\frac{\partial E_n}{\partial B} \right) f\left(E_n - \mu\right) \text{ and } \chi = \frac{\partial M}{\partial B} \tag{1}$$

where n stands for the electronic state with corresponding energy E_n, $f(x)$ is the Fermi distribution function, and μ is the chemical potential of the system determined from the number of the electrons confined in the NR: $N = \sum_n f\left(E_n - \mu\right)$.

The magnetic field strength's change results in crossings between lowest subsequent energy levels of NRs and oscillations in the magnetization (the Aharonov–Bohm oscillations). At low temperatures the aperiodic oscillations of magnetization generate delta-like positive peaks in the ring's DMS [3]. At the same time the peaks' positions and amplitudes strongly depend on the actual geometrical and material parameters of NRs such as effective radii, heights, material content, etc. In this paper we concentrate only at the first peak (which is the most visible in experiments). This peak corresponds to the crossing between energy states E_0 and E_1. One should notice that the electronic energies E_n of NRs can be characterized by a set of parameters: $\{R,h,\xi,\ldots\}$, where R, h, ξ represent characteristic radius, height, anisotropy coefficient (see equation 3), etc. The geometrical and material parameters' dispersions in ensembles of NRs are described by a multidimensional distribution function $P(R,h,\xi,\ldots)$ which gives the number of NRs dN with the values of $\{R,h,\xi,\ldots\}$ inside the domain $\{[R,R+dR]$, $[h,h+dh]$, $[\xi,\xi+d\xi]$,...$\}$ as $dN = P(R,h,\xi,\ldots)\, dRdhd\xi\ldots$In this study we assume that the NR parameters in typical structures are distributed according to the non-correlated normal distribution $P(R,h,\xi,\ldots) = P_G(R)P_G(h)P_G(\xi)\ldots$, where the standard normal distributions are presented by the probability density function $P_G(x) = A \cdot G[(x-x^0)/\Delta x]$, A stands for the normalization coefficient, x^0 is an mean value and Δx is the standard deviation of the parameter x, and G[y] is the Gaussian function. With including the parameters' variations in the ensemble of the rings we can write the following expression for the experimental meaningful (average) DMS:

$$\overline{\chi} = \int P(\{x_i\})\chi(\{x_i\}) \prod_i dx_i \tag{2}$$

where $\{x_i\}$ represents set of the appropriate parameters.

To bridge NR parameters' variations and DMS changes in this paper we adopt the mapping procedure in constructing a three-dimensional model of a NR as it was described in Ref. [4]. For an asymmetric (wobbled) *InAs/GaAs* NR we first assume that the ring was grown on a substrate parallel to the x-y plane (see inset in figure 1). Using known experimental data obtained from AFM (atomic force microscopy) and X-STM (cross-sectional scanning tunneling microscopy) [1,2] we model the geometry of the ring by mapping the height of the ring $h(x,y)$ with the following function:

$$h(x,y) = h_0 + \gamma_0^2 R_r^{-2}\left[h_r\left(1 + \xi\frac{x^2-y^2}{x^2+y^2}\right) - h_0 \right] \cdot \frac{R_r^2 - \left(\sqrt{x^2+y^2} - R_r\right)^2}{\left(\sqrt{x^2+y^2} - R_r\right)^2 + \gamma_0^2}; \sqrt{x^2+y^2} \le R_r$$

$$h(x,y) = h_\infty + \gamma_\infty^2\left[h_r\left(1 + \xi\frac{x^2-y^2}{x^2+y^2}\right) - h_\infty \right]\left[\left(\sqrt{x^2+y^2} - R_r\right)^2 + \gamma_\infty^2\right]^{-1}; \sqrt{x^2+y^2} > R_r \tag{3}$$

where h_0, h_r, h_∞ stand correspondingly for the height at the center of the ring, at the rim of the ring (when $x^2 + y^2 = R_r^2$), and far away from the center of the ring; γ_0 and γ_∞ respectively determine the inner and outer slope near the rim. The parameter ξ defines the anisotropy of the ring height in the (x, y) plane. Three-dimensional confinement potential for electrons can be found from the composition and geometry dependent conducting band profile: $V(x,y,z) = \Delta E_C \cdot\{1\text{-}1/4[1+\tanh(z\text{-}z_0/a)][1\text{-}\tanh(z\text{-}h(x,y)/a)]\}$, where ΔE_C is the electronic band offset for the ring *InAs/GaAs* structures. The slope of the potential and the range of the potential change at the boundaries of the object is controlled by the

parameter a. The potential is used to define the mapping function $M(x,y,z) = 1\text{-}V(x,y,z)/\Delta E_C$. The mapping function reproduces experimental information about geometry (shape) and position dependent composition of the ring. Using $M(x,y,z)$ we model the position dependent band gap $E_g(x,y,z)$, spin-orbit interaction splitting $\Delta(x,y,z)$, and the effective mass at the bottom of the conducting band $m(x,y,z)$. Those functions we conventionally use for the effective one-electronic-band Hamiltonian (energy and position-dependent electron effective mass and g-factor approximation) [5,6]. The realistic semiconductor material parameters for the *InAs/GaAs* heterostructure with complex strained composition are used according to [4]. To determine the single electron magnetic response of an isolated NR we calculate the energy states of the ring with a predefined set of parameters $\{R_r,h_0,h_r,h_\infty,\xi,\gamma_0,\gamma_\infty,a,\Delta E_C\}$. The energy states are found by the nonlinear iterative method (see for instance [6] and references therein) using the COMSOL Multiphysics package (www.comsol.com). As an example of our simulation results we present in figure 1 two lowest energy states and DMS of the single electron *InAs/GaAs* NR when: $\{R_r = 9$ nm, $h_0 = 1.6$ nm, $h_r = 3.6$ nm, $h_\infty = 0.0$ nm, $\xi = 0.15$, $\gamma_0 = 3.0$ nm, $\gamma_\infty = 5$ nm, $a = 0.5$ nm, $\Delta E_C = 0.44$ eV$\}$.

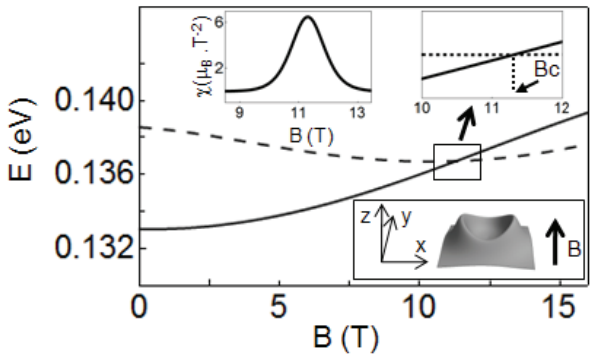

Figure 1. Energy states and DMS (upper left inset, μ_B stands for the Bohr magneton) of a wobbled nano ring. All explanations see in the text.

We stress that at low temperatures the DMS peak position and amplitude are obviously defined by the properties of two lowest energy states as functions on the magnetic field. Near the crossing point (B_C) we can approximate the electronic energies: $E_{0,1}(B) \approx E_0(B_C) + C_{0,1}(B - B_C)$ (see the upper right inset of figure 1). With this approximation the DMS of a single electron NR may be written as

$$\chi(B,T) \approx \frac{(C_1 - C_0)}{2k_B T}\left\{\frac{C_1 \exp(\delta)}{[1+\exp(\delta)]^2} - \frac{C_0 \exp(-\delta)}{[1+\exp(-\delta)]^2}\right\} \tag{4}$$

where $\delta = (C_1\text{-}C_0)\cdot(B\text{-}B_C)/2k_BT$, T stands for the temperature, and k_B is the Boltzmann constant.

Our mapping method allows us efficiently and economically to simulate energy states of NRs by varying parameters within a wide range. For reason of clarity in this short paper we restrict our consideration only to variations of the DMS peak caused by the rim radius R_r dispersion. Other parameters we assume to be fixed as for the individual ring above. To connect the DMS peak variations and changes of R_r on the base of our simulation experience and results we propose to use the following type of functions to describe the crossing point B_C and coefficients $C_{0,1}$ dependencies on R_r:

$$B_C = a_B + b_B \cdot R_r^{\beta_B};\ C_0 = a_0 + b_0 \cdot R_r^{\beta_0};\ C_1 = a_1 + b_1 \cdot (R_r - \beta_1)^{-1} \tag{5}$$

where $a_{B,0,1}$, $b_{B,0,1}$, and $\beta_{B,0,1}$ are parameters to be fitted by use of our simulation results when only R_r has been varied within the interval 6.5 ÷ 12.5 nm. The parameters have been found to be (in appropriate SI units): $a_B = 1683.9$, $b_B = 0.92$, $\beta_B = -2.24$; $a_0 = 9.6\times10^{-3}$, $b_0 = 7.4\times10^{-3}$, $\beta_0 = 9.3\times10^{-2}$; $a_1 = -1.9\times10^{-5}$, $b_1 = 7.3\times10^{-5}$, $\beta_1 = 6.15$. The fitted expressions (5) and equation (4) we use to simulate the average DMS:

$$\overline{\chi}_R(B,T) = \int P(R_r)\chi(B,T;R_r)dR_r \tag{7}$$

Figure 2 shows the simulation results for the DMS of an individual ring with R_r = 9 nm and the DMS averaged within the ensemble of rings with the mean value R^0_r = 9 nm and standard deviation ΔR_r = 0.5 nm. The averaged DMS peak is much lower than the individual ring's DMS. Without including the radius variations, the calculated amplitude of the individual NR DMS's peak sharply increases with decreasing temperature. At the same time the averaged within the ensemble of NRs DMS's demonstrates temperature stable behaviour. This was observed experimentally in [1].

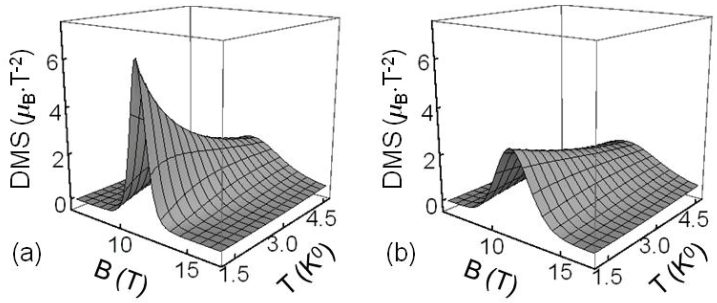

Figure 2. Dependence of the differential magnetic susceptibility on magnetic field and temperature: (a) a single ring; (b) DMS averaged within an ensemble of the rings.

In short conclusions the simulations showed that the DMS amplitude is sensitive to the exact geometry and composition of semiconductor nano rings. We theoretically demonstrated a small temperature effect on averaged DMS of ensembles of the rings. It follows from this study that experimental investigations of the magnetic response of specially designed ensembles of NRs can be potentially useful for further fabrication of systems with principally new magnetic properties.

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