Proc. Natl. Conf. Theor. Phys. **37** (2012), pp. 37-41

EFFECT OF SIZE DISPERSION ON THE AVERAGED MAGNETIC SUSCEPTIBILITY OF ENSEMBLES OF SEMICONDUCTOR QUANTUM RINGS

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Abstract. *In this paper we theoretically study the effect of size dispersion on the averaged magnetic susceptibility of ensembles of asymmetrical InGaAs/GaAs quantum rings. Using our mapping method, we are able to calculate the magnetic susceptibility of individual ring with fixed geometrical parameters. Considering dispersion of the ring's rim radius, we simulate homogeneous and inhomogeneous broadening of the averaged magnetic susceptibility of the ensembles of semiconductor quantum rings. The averaged magnetic susceptibility of the rings' ensembles demonstrates stable temperature dependence. Our simulation results clearly explain the experimental observations.*

I. INTRODUCTION

Recent experiments on self-assembled InGaAs/GaAs quantum rings demonstrate possibility to control geometrical and material parameters of those semiconductor nano-objects [1, 2, 3]. The topological quantum effects for electrons confined in a ring (the Aharonov-Bohm effect) result in unusual behavior of the magnetic susceptibility of the ring [3, 4]. The appearance of the positive peak in the magnetic susceptibility at low temperatures has to be addressed to the crossing between the two lowest-energy states of the electron confined in the ring. The experimental results demonstrated a stable temperature dependence of the magnetic susceptibility [2]. In this study using our mapping method [5, 6] we address the issue of the temperature dependence of the magnetic susceptibility of ensembles of asymmetrical InGaAs/GaAs quantum rings. Considering dispersion of the ring's rim radius, we calculated the averaged magnetic susceptibility of the ensembles of the rings. The averaged magnetic susceptibility of the rings' ensembles demonstrates stable temperature dependence unlike the magnetic susceptibility of individual ring. Our simulation results are in good agreement with experimental data.

II. THEORY

For an asymmetric InGaAs/GaAs quantum rings we first assume that the ring was grown on a substrate on the xy plane. Using 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:

$$h(x,y)=\begin{cases} h_0+\left[h_r\left(1+\xi\frac{x^2-y^2}{x^2+y^2}\right)-h_0\right]\frac{\gamma_0^2}{R_r^2}\frac{R_r^2-(\sqrt{x^2+y^2}-R_r)^2}{(\sqrt{x^2+y^2}-R_r)^2+\gamma_0^2}, & \sqrt{x^2+y^2}\le R_r,\\ h_\infty+\left[h_r\left(1+\xi\frac{x^2-y^2}{x^2+y^2}\right)-h_\infty\right]\frac{\gamma_\infty^2}{(\sqrt{x^2+y^2}-R_r)^2+\gamma_\infty^2}, & \sqrt{x^2+y^2}>R_r, \end{cases} \tag{1}$$

where R_r is the ring's rim radius, h_0, h_r, and h_∞ correspondingly stand for the height at the center of the ring, at the rim, and far outside of the ring. γ_0 and γ_∞ respectively determine the inside and outside slopes near the ring's rim. The parameter ξ defines the anisotropy of the ring height on the xy plane. The three-dimensional smooth confinement potential for electrons is presented:

$$V(x,y,z) \;=\; \Delta E_c\left\{1-\frac{1}{4}\left[1+\tanh\left(\frac{z}{a}\right)\right]\times\left[1-\tanh\left(\frac{z-h(x,y)}{a}\right)\right]\right\}, \tag{2}$$

where ΔE_c is the electronic band offset for the InAs/GaAs ring structures, parameter a control the slope and range of the potential change at the boundaries of the ring. Using the potential (2) we define the mapping function:

$$M(x,y,z)=1-\frac{V(x,y,z)}{\Delta E_c}. \tag{3}$$

This function accumulates experimental information about the ring shape and it allows us to model the position dependent band gap $E_g(\mathbf{r})$, spin-orbit splitting $\Delta(\mathbf{r})$, and the electron effective mass at the bottom of the conducting band $m_b(\mathbf{r})$ as the following expressions:

$$\begin{aligned} E_g(x,y,z)&=E_g^{in}M\left(x,y,z\right)+E_g^{out}\left[1-M\left(x,y,z\right)\right],\\ \Delta(x,y,z)&=\Delta^{in}M\left(x,y,z\right)+\Delta^{out}\left[1-M\left(x,y,z\right)\right],\\ m_b(x,y,z)&=m_b^{in}M\left(x,y,z\right)+m_b^{out}\left[1-M\left(x,y,z\right)\right]. \end{aligned} \tag{4}$$

Energy states of a single electron confined in the ring can be obtained in the one band approximation by solving the nonlinear Schrödinger equation [7, 8] :

$$\hat{H}(E,\mathbf{r})F(\mathbf{r})=EF(\mathbf{r}), \tag{5}$$

with the effective energy-dependent Hamiltonian

$$\hat{H}(E,\mathbf{r})=\frac{1}{2}\mathbf{\Pi_r}\frac{1}{m(E,\mathbf{r})}\mathbf{\Pi_r}+\frac{\mu_B}{2}g(E,\mathbf{r})\sigma\cdot\mathbf{B}+V(\mathbf{r}), \tag{6}$$

where $\mathbf{\Pi_r}=-i\hbar\nabla_\mathbf{r}+e\mathbf{A}(\mathbf{r})$ is the electron momentum operator, $\nabla_\mathbf{r}$ is the spatial gradient, $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field $\mathbf{B}=\nabla\times\mathbf{A}$, σ is the vector of the Pauli matrices, μ_B is the Bohr magneton, $m\left(E,\mathbf{r}\right)$ is the energy and position dependent electron effective mass, $g\left(E,\mathbf{r}\right)$ is the energy and position dependent Landé factor, and e is the elementary charge.

To determine the magnetization M (total magnetic moment) and magnetic susceptibility χ for an isolated quantum 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 magnetic susceptibility of the ring are written as the following [9]

$$M=\sum_n\left(-\frac{\partial E_n}{\partial B}\right)f\left(E_n-\mu\right),\chi=\frac{\partial M}{\partial B}, \tag{7}$$

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 electrons confined in the quantum ring.
The magnetic field strength's change results in crossings between two lowest energy levels of quantum rings and positive peaks in the ring's magnetic susceptibility [2]. The peaks' positions and amplitudes strongly depend on the actual geometrical parameters of quantum rings such as effective radii and heights, etc. In this paper we concentrate only at the first peak which corresponds to the crossing between two lowest energy states E_0 and E_1. The magnetic susceptibility 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: $E_{0,1}(B) = E_0(B_C) + C_{0,1}(B - B_C)$. With this approximation the magnetic susceptibility of a single electron ring can be expressed:

$$\chi = -\frac{(C_0 - C_1)}{2k_B T}\left\{\frac{C_0 \exp(-\delta)}{[1+\exp(-\delta)]^2} - \frac{C_0 \exp(\delta)}{[1+\exp(\delta)]^2}\right\}, \tag{8}$$

where

$$\delta = \frac{(C_0 - C_1)\,(B - Bc)}{k_B T}.$$

T is the temperature, and k_B is the Boltzmann constant.
With including the variations of ring' radius in the ensemble we can write the following expression for the averaged magnetic susceptibility:

$$\overline{\chi}(B,T) = \int\limits_{R_r} P(R_r)\chi(B,T,R_r)dR_r, \tag{9}$$

where $P(R_r)$ is the standard normal distributions.
To connect the magnetic susceptibility peak changes and variations of rim radius R_r, according to our simulation experience, 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:

$$B_C(R_r) = a + b.R_r^{\alpha}; C_0(R_r) = a_0 + b_0.R_r^{\alpha_0}; C_1(R_r) = a_1 + b_1 R_r^{\alpha_1} \tag{10}$$

where $a, a_{0,1}$, $b, b_{0,1}$, α, and $\alpha_{0,1}$ are parameters to be fitted by use of our simulation results when only R_r has been varied within the interval $10.5 \div 12.5$ nm. We use the fitted expressions (10) and equations (9) to simulate the average magnetic susceptibility of ring's ensemble.

III. SIMULATION RESULTS AND DISCUSSION

To determine the single electron magnetic susceptibility of an isolated quantum ring we calculate the energy states of the ring with a predefined set of geometrical parameters. The realistic semiconductor material parameters for the InAs/GaAs heterostructure with complex strained composition are used according to Refs. 10, 11. Geometrical parameters are chosen to be $h_0 = 1.6$ nm, $h_r = 3.6$ nm, $h_\infty = 0$ nm, $\xi = 0.2$, $\gamma_0 = 4.5$ nm, $\gamma_\infty = 2.0$ nm, $a = 0.5$ nm. In our simulations the parameter R_r is varied within the range from 10.5 nm to 12.5 nm. The energy states are found by the nonlinear iterative method (see for instance [12] and references therein) using the Comsol Multiphysics package [13]. Values of

$B_C(R_r)$ and $C_{0(1)}(R_r)$ are reproduced from the calculation results. According to our experience, the best fit can be achieved with the fitting parameters $a = 55.13$, $a_0 = 14.2\times10^{-4}$, $a_1 = 22.46 \times 10^{-4}$, $b = -6.25$, $b_0 = -1.5 \times 10^{-4}$, $b_1 = 12.47 \times 10^{-4}$,$\alpha = 0.77$, $\alpha_0 = 0.75$, $\alpha_1 = 0.206$ (in appropriate SI units). It is clear from Fig.1.(a)-(c) that the fitting functions of crossing point $B_C(R_r)$ and coefficients $C_{0(1)}(R_r)$ accurately reproduce results of our direct simulation within the chosen range of variation of the parameter. Substituting $B_C(R_r)$ and $C_{0(1)}(R_r)$ from Eq. (10) with above fitting parameters into Eqs. (8),(9), we now able to simulate the averaged magnetic susceptibility for the dispersive ensemble of quantum rings and compare with magnetic susceptibility of a single ring. Figure 2 shows

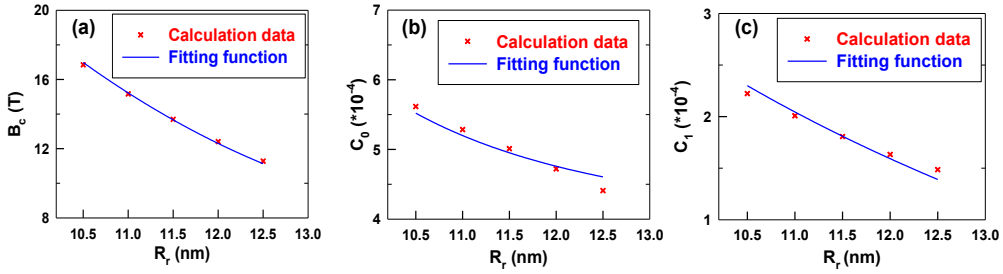

Fig. 1. Dependencies of (a) crossing point B_C, (b) coefficient C_0 and (c) coefficient C_1 on the ring's rim radius R_r

results of our simulations for the temperature and magnetic field dependence of magnetic susceptibility of an individual $InGaAs/GaAs$ ring with $R_r = 11.5$ nm and the same value averaged within the ensembles of the rings with the mean value $\bar{R}_r = 11.5$ nm, when the standard deviation is taken to be $\triangle R_r = 0.5$ nm. Clearly, for the individual quan-

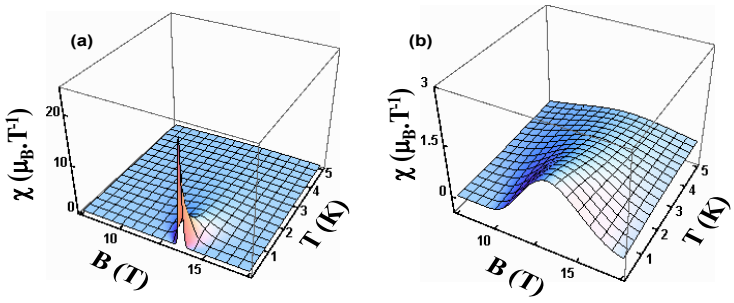

Fig. 2. Dependence of the magnetic susceptibility on the temperature and magnetic field for (a) individual ring ($R_r = 11.5$ nm) and (b) ring ensemble ($\bar{R}_r = 11.5$ nm, $\triangle R_r = 0.5$ nm)

tum ring at very low temperatures the magnetic susceptibility demonstrates a very sharp symmetrical positive peak (Fig. 2(a)) near the crossing point B_C. The amplitude of the magnetic susceptibility peak is controlled by the temperature fluctuations (homogeneous broadening). The peak become wider and disappear very rapidly when the temperature

increases. This is in contrast to the experimental data from Ref. 2, where the relatively wide peak reveals itself even when the temperature increases. The temperature stable wide peak of the magnetic susceptibility can be explained by the radius dispersion in the ring ensembles. To demonstrate this, in Fig. 2(b)we present the magnetic susceptibility of the ensemble of the rings. Obviously, the peak of the magnetic susceptibility demonstrates the temperature stable behavior, which has to be attributed to size dispersion in the ensemble (inhomogeneous broadening) and this clearly explains the experimental results reported in Ref. 2.

In short conclusion, our simulations showed that the averaged magnetic susceptibility peak of ring's ensembles is much lower than the individual ring's magnetic susceptibility peak. We theoretically demonstrated a stable temperature dependence on the averaged magnetic susceptibility of ring's ensembles. It follows from this study that experimental investigations of the magnetic response of ensembles of semiconductor quantum rings can be potentially useful for further fabrication of systems with new magnetic properties.

ACKNOWLEDGMENT

We would like to thank National Foundation for Science and Technology Development (NAFOSTED) for financial support. We would like to thank Solid State Physics Lab, Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University where a part of numerical calculations was done.

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Received 30-09-2012.