行政院國家科學委員會專題研究計畫期中（第二年）報告

半導體奈米元件的軌道與電子自旋磁性
Orbital and spin magnetism in semiconductor nano-objects

計畫編號：NSC 97-2112-M-009-012-MY3

執行期限：98 年 08 月 1 日至 99 年 7 月 31 日

主持人：霍斯科 (O.Voskoboynikov) 教授 交通大學電子工程系暨電子研究

一 摘要 (Abstract)

英文

This report summarizes major results obtained from the second year program of the ”Orbital and spin magnetism in semiconductor nano-objects” project. Two directions of the research have been pursued, as described in detail in the report: problems of a general description of the magneto-optics of three dimensional arrays of semiconductor nano-objects including magneto-excitonic effects and the temperature stable unusual diamagnetism of ensembles of semiconductor nano-rings generated by the rings' geometrical and material parameters’ dispersions. In addition we theoretically studied magneto-optics of three-dimensional arrays of double quantum dot molecules. Several publications were performed based on this year’s results.

中文

這份報告總結了"半導體奈米元件的軌道與電子自旋磁性"第二年計劃的主要成果, 我們兩個的研究方向如下所述: 三微陣列的半導體奈米物體的磁光學通用描述問題, 包含激子的磁場效應; 以及具有環狀幾何形狀與材料特性的半導體奈米環, 其整體的溫度低相關的特殊反磁性. 此外, 我們進行理論分析三微陣列雙量子點分子的磁光特性, 此年的研究成果已經成功刊登在數個期刊上.

二 Magneto-optics of three dimensional arrays of semiconductor nano-objects including magneto-exitonic effects.

The hybrid discrete-continuum model (derived by us recently in *PRB* 2005, 2006, 2009) makes it possible to simulate complex optical properties of three dimensional arrays (ensembles) of semiconductor nano-objects embedded in a dielectric matrix. Each embedded nano-object gets represented by a single discrete dipole, characterized by a bare excess polarizability. This polarizability includes the screening by the surrounding continues dielectric medium. To obtain the collective optical response one should solve the system of equations similar to known from the discrete-dipole approximation. The method allows us to simulate the collective magneto-optical response the nano-objects of arbitrary random shapes and positions within the arrays. Using the method we theoretically studied the optical response of three-dimensional *InAs/GaAs* quantum dot multilayered structures (Fig. 1). First we defined the optical response of an isolated layer of embedded quantum. Then using the propagation-matrix approach we express the amplitudes of incident, reflected and transmitted electromagnetic waves in a multilayered structure by the reflection and transmission coefficients of the isolated layers. We studied the overall reflectance and transmittance dependencies on the number of layers and distance between consecutive layers. The reflectance of the structures including several layers for s-polarized light is shown in Fig. 2. The peaks in the reflectance relate to the allowed optical transitions in the quantum dots. Clearly, for a single layer the reflectance is weak. However the reflectance still reproduces important information on quantum mechanics of individual quantum dots. When the number of the layers in the structure increases the overall reflectance of the structure considerably enhances (Fig. 2). For large enough distance between the layers *d* the interference becomes significant and this leads to the appearance of the periodical peaks in the reflectance. The dependence of the overall reflectance on the transition energy and distance *d* for the structure consisting of five layers is presented in Fig. 3. The figure shows that the interference effects become significant for certain distances between layers in the structures.

We also simulated the magneto-biexciton systems confined in the asymmetrical wobbled *InAs/GaAs* nano-rings, using a smooth three dimensional confinement potential which realistically describes electronic properties of the rings. In our calculation, we used the Hartree approximation to calculate the self-consistent energy for exciton and biexciton confined in the system. We simulated recombination energy, binding energy and their diamagnetic shifts and compare those results with experimental data obtained from the magneto-photoluminescence measurement. We found that using the realistic geometry and composition of the asymmetric nano-ring in our simulations we are able to reproduce experimental data with good accuracy and explain the experimentally obtained difference in diamagnetic shifts of excitons and biexcitons (see Fig.4 and Fig. 5) .

三 Temperature stable unusual diamagnetism in semiconductor nano-rings.

Three-dimensional topological quantum effects (similar to the Aharonov-Bohm effect) for electrons confined in a nano-ring result in unusual behavior of the differential magnetic susceptibility of the ring containing only a single electron: appearance of the positive peak in the differential magnetic susceptibility at low temperatures which has to be addressed to the Aharonov-Bohm crossing between two lowest energy states of the electron confined in the ring (Fig. 6). The actual experimental height of the peak and its temperature dependence were found in contradiction to the theoretical description performed recently by the authors. Unlike in the theoretical simulation results the experimental peak demonstrated a negligible temperature effect. We stress that the inherent property of the contemporary semiconductor self-assembled nano-objects is their geometrical and material parameters' dispersions. One should notice that the electronic energies E_n of nano-rings can be characterized by a set of parameters: $\{R,h,\xi,\ldots\}$, where R, h, ξ, .. represent characteristic radius, height, anisotropy coefficient, etc. 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-rings. Our mapping method allows us efficiently and economically to simulate energy states of nano-rings by varying parameters within a wide range. The simulations showed that the differential magnetic susceptibility amplitude is sensitive to the exact geometry and composition of semiconductor nano rings. We theoretically demonstrated a small temperature effect on averaged differential magnetic susceptibility of ensembles of the rings (Fig. 7). This inhomogeneous broadening is shielding the homogeneous one at the low temperature regime. It follows from this study that experimental investigations of the magnetic response of specially designed ensembles of nano-rings can be potentially useful for further fabrication of systems with principally new magnetic properties.

四 Magneto-optics of three-dimensional arrays of double quantum dot molecules

We considered impact of the coherent manipulation of excitonic states in the double vertical lens-shaped circular quantum dot molecules on the effective permittivity of three-dimensional arrays made from those nano-objects. The manipulation is performed for *InAs/GaAs* quantum dot molecules assembled from the dots with substantially different diameters and when an external magnetic field is along the system's growth direction (Fig. 8). The influence of the surrounding semiconducting matrix upon the polarizability of embedded quantum dot molecules has been investigated using a hybrid discrete/continuum model. We first calculated transition energies and corresponding overlap integrals (those represent the optical transition matrix element). Certain optical transitions are allowed when the corresponding three-dimensional overlap integral cannot be vanished. The magnetic field dependencies of two lowest allowed optical transitions in our quantum dot molecule with relatively large distance between the dots (20 nm, the tunnel coupling between dots is weak) are shown in Fig. 8. Using the bare embedded polarizability we can write an effective permittivity for the array of the quantum dot molecules according to the Clausius – Mossotti relation. To illustrate impact of the quantum mechanical properties of individual *InAs/GaAs* quantum dot molecules on the overall optical characteristics of arrays made from them we show in Fig. 9 and Fig. 10 the real and imaginary parts of the corresponding diagonal component of the effective permittivity tensor. The peak in Fig. 10 corresponds to the crossing of the energies of two transitions (Fig. 8). In the crossing point they contribute in resonance simultaneously and this increases the response by the factor of two. Obviously, small damping parameter Γ ensures a clear reflection of the quantum mechanical properties of an individual quantum dot molecule in the collective magneto-optical response of the array of quantum dot molecules. We should stress, that even for relatively large Γ = 1meV (that we use in our simulations) the quantum mechanics of the quantum dot molecules clearly shows itself from the magneto-optical data. The simulation results show that the change in the quantum mechanical properties of the quantum dot molecules can be observable by monitoring the changes of the magneto-optical characteristics of three-dimensional arrays made from these nano-objects.

Publications:

1. C. M. J. Wijers and O. Voskobyonikov, "Magnetic qubit in a non-magnetic semiconductor quantum dot molecule", invited and submitted to the Journal of Computational and Theoretical Nanoscience, planed to be published in September 2010.
2. L. M. Thu, W. T. Chiu and O. Voskoboynikov, " Temperature stable positive magnetic susceptibility of semiconductor wobbled nano rings", accepted to Journal of Physics: Conference Series, to be published in 2010.
3. L.M. Thu , O. Voskoboynikov, " Computer simulation of the non-uniform and anisotropic diamagnetic shift of electronic energy levels in double quantum dot molecules", Computational Materials Science, Available online 8 April 2010.
4. O. Voskoboynikov, "Hybrid Model for Simulation of Magneto-Optical Response of Layers of Semiconductor Nano-Objects", International Journal for Multiscale Computational Engineering, vol. 8, no. 2. pp-153-164, (2010).
5. Thu Le Minh and O. Voskoboynikov," Simulation of an Asymmetrical Nano Ring by Mapping of the Realistic Electronic Confinement Potential", AIP Conference Proceedings, vol. 1233, pp. 952-957, May. (2010). (SCI).
6. Thu Le Minh and O. Voskoboynikov," Unusual Diamagnetism in Semiconductor Nano-Objects", Physics Procedia, vol. 3, no. 2, pp. 1133-1137, Jan. (2010). (SCI).
7. L. M. Thu, W. T. Chiu, Shao-Fu Xue, and O. Voskoboynikov, "Binding energy of magneto-biexcitons in semiconductor nano-rings", Physics Procedia vol. 3, no. 2, pp. 1149-1153, Jan. (2010). (SCI).
8. Thu Le Minh and O. Voskoboynikov, "Magneto-optics of two dimensional arrays of semiconductor quantum dot molecules", Physica E, vol. 42, no. 4, pp. 887-890, Feb. (2010) (SCI).
9. Thu Le Minh and O. Voskoboynikov, “Magneto-optics of layers of double quantum dot molecules”, Physical Review B, vol. 80, no. 15, 155442-1-12, Nov. 2009. (SCI).
10. L. M. Thu and O. Voskoboynikov, " Optical response of quantum dot multilayer structures", Presentation in the QD2010, Nottingham, April, 2010.
11. L. M. Thu, W. T. Chiu and O. Voskoboynikov, " Temperature stable positive magnetic susceptibility of semiconductor wobbled nano rings", Presentation in the QD2010, Nottingham, April, 2010.
12. L. M. Thu and O. Voskoboynikov, ” Simulation of an Asymmetrical Nano Ring by Mapping of the Realistic Electronic Confinement Potential”, oral presentation in the ISCM II and EPMESC XII, Hong Kong – Macau, Nov.- Dec., 2009.
13. L. M. Thu and O. Voskoboynikov, "Computer simulation of the non-uniform and anisotropic diamagnetic shift of electronic energy levels in double quantum dot molecules", the 5th Conference of the Asian Consortium on Computational Materials Science, Vietnam, Sep., 2009.

Figures:

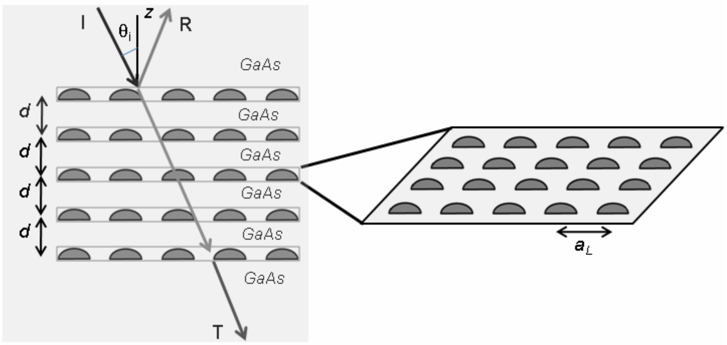

Fig. 1. Scheme of the quantum dot multilayer structure.

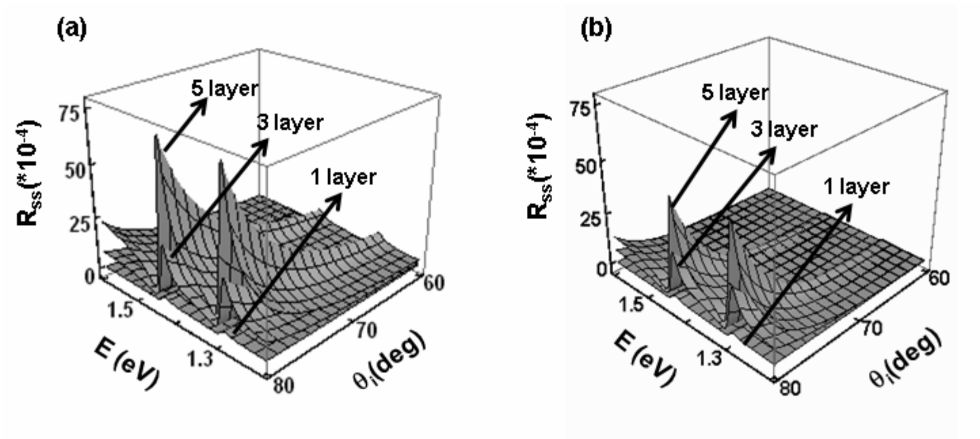

Fig. 2. Reflectance of the quantum dot multilayered structures as a function on the transition energy and angle of incidence: (a) d = 10nm and (b) d = 50nm.

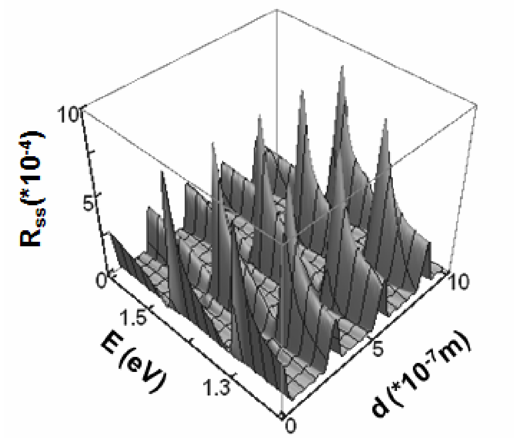

Fig. 3. Reflectance of the quantum dot multilayered structure consisting of five layers as a function on the transition energy and distance between the consecutive layers.

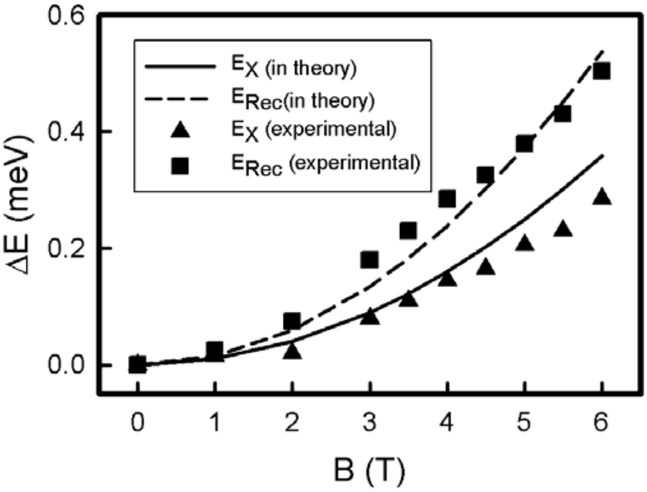

Fig. 4. Diamagnetic shifts of the excitonic energies confined in a nano-ring.

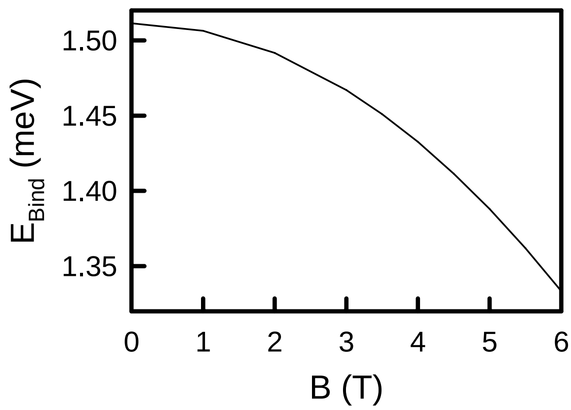

Fig. 5. Biexciton binding energy as a function on magnetic field for a nano-ring.

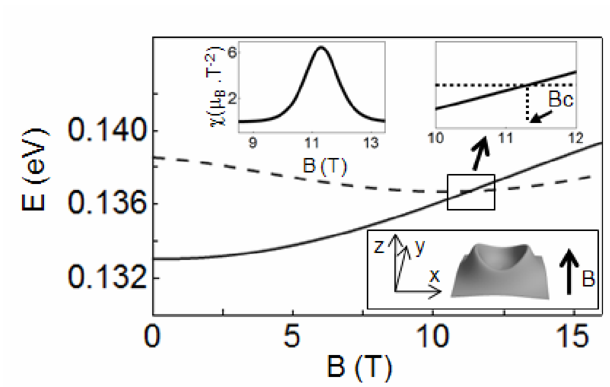

Fig. 6. Energy states and differential magnetic susceptibility (upper left inset, μ_B stands for the Bohr magneton) of a wobbled nano ring. All explanations see in the text.

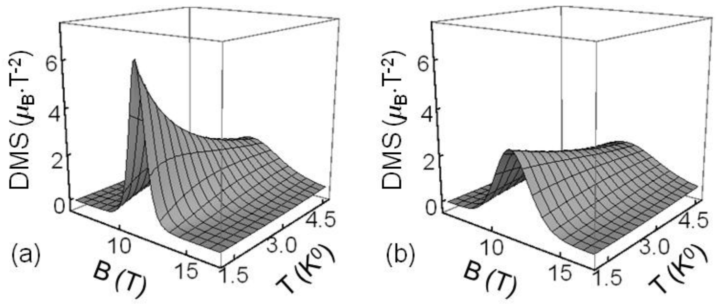

Fig. 7. Dependence of the differential magnetic susceptibility (DMS) on magnetic field and temperature: (a) a single ring; (b) differential magnetic susceptibility averaged within an ensemble of the rings.

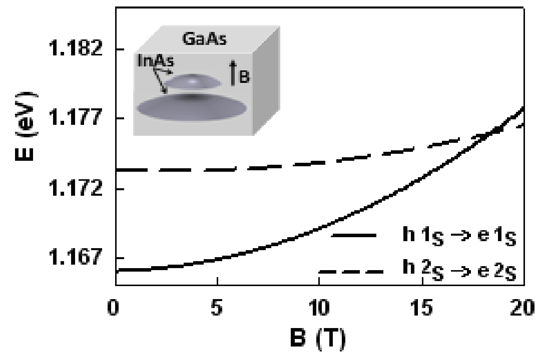

Fig. 8. Lowest transition energies as functions of the magnetic field for the asymmetric quantum dot molecule.

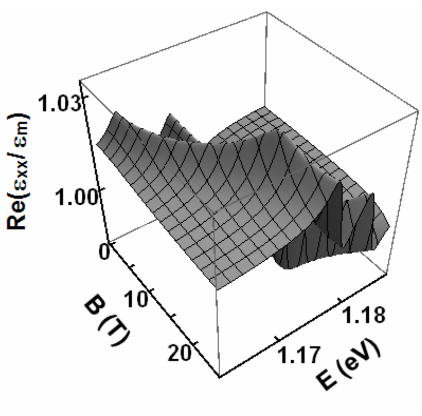

Fig. 9. Normalized real part of the effective permittivity of the array of quantum dot molecules.

.

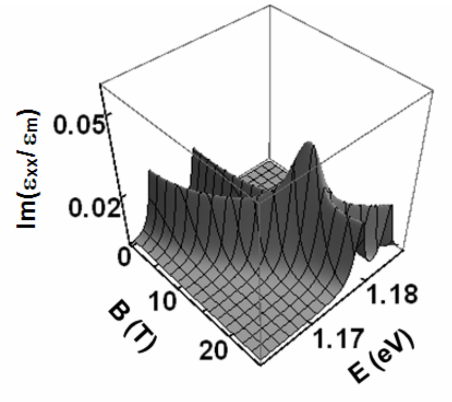

Fig. 10. Normalized imaginary part of the effective permittivity of the array quantum dot molecules.