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奈米結構合成材料的磁光效應(1/3)

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行政院國家科學委員會專題研究計畫期中（第一年）報告

奈米結構合成材料的磁光效應

Magneto-Optics of Nano-Stuctured Composite Materials

計畫編號：94-2112-M-009-037-

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一 摘要 (Abstract)

英文

This report summarizes the major results obtained from the first year program of the ”Magneto-Optics of Nano-Stuctured Composite Materials” project. Two directions of research have been pursued, as described in detail in the report: problems of the influence of embedding upon the optical response of nano-objects and the first stage of analysis of the influence of the surface of the capped system. In addition we demonstrate an interesting opportunity to drive dynamically coupled electronic states in vertically stacked double *InAs/GaAs* quantum dot molecule (relocate electronic wave functions from one dot to another) by applying external magnetic field. Several publications were performed based on this year’s results.

中文

這份報告總結了”奈米結構合成材料的磁光效應”計畫的初年主要的研究成果，我們兩個研究方向分別是：嵌埋對奈米物體光響應的影響、不同覆蓋材料對表面的影響的初步分析。此外我們藉著施加磁場，成功驅動’垂直堆疊雙砷化銦/砷化鎵量子點’的電子能階耀動(電子波函數由其中一個量子點移動到另一個)。今年的研究成果已成功發表數篇論文。

二 Influence of Embedding upon Optical Response Nano-Objects and Influence of Surface upon Optical Response Embedded Nano-objects

At the start of the project we had published already about the magneto-optical response of single layers of free floating nano-objects (nano rings), where we have shown that the full optical response can be obtained by adding the quantum mechanical contribution of a limited number of transition energies to a continuum electrostatic response. The continuation of this research into the direction of the full optical response of a regular capped array of nano-objects (see Fig. 1) requires full knowledge about the influence of embedding upon this response. This asks for investigation of both the continuum local and discrete non-local aspects of the hybrid model. We have investigated the fundamental aspects of the connectivity between polarizability and dielectric constant descriptions and closely examined the consequences of source based and source free descriptions in electromagnetism as is required by boundary condition type of solutions. On the basis of these insights the hybrid model could be linked to the full macroscopic continuum solution of dielectric spheres and ellipsoids. It turns out that the transition of this local continuum approach towards the required non-local discrete description, takes place through the transformation of the dressed polarizability, as comes out from those calculations, into a bare excess polarizability and an intracellular transfer tensor. In the discrete description now intercellular (between nano-objects) transfer tensors can be used to describe the collective optical response (Fig. 2). This is the unique advantage of this hybrid method, not available to common continuum models. All tensors (

intracellular and intercellular) are found to be screened by the dielectric constant of the embedding medium. The bare polarizability in contrast is simple and shows no trace of screening at all. To this bare excess polarizability the dynamical quantum mechanical contribution, responsible for the magnetic field dependence, has to be added. Using this scheme we calculated the optical response of several nano-object systems and came to the conclusion that embedding only slightly weakens the optical response, by that all physical and technologically relevant structure in the frequency dependent signal gets relatively enhanced by one to two orders of magnitude (Fig. 3 -Fig. 5).

As a sideline research project we have derived improved expressions for both the polarizability and electric fields of general oblate ellipsoidal bodies. The disadvantage of existing treatments about this subject is that they do not offer directly usable expressions for the external electric field and that they are not compatible with the derivation of the standard case: the dielectric sphere. We have cured both shortcomings by developing a much simpler description using a new set of basis functions in Cartesian coordinates. The external field expression is indispensable to correct in the future for the short range discrepancies in the present hybrid description.

In the hybrid model description of embedded nano-objects, the incorporation of the surface of the capping layer covering the embedded objects is the last stage to arrive at (easily) measurable results. The first stage of this research deals with the response of the dipole strength's below the surface. To that end a transmitted dipole for the outer area and a reflected (mirror) dipole for the inner area are required. The dependency of these two additional dipoles upon surface and original dipole has been obtained.

三 Dynamically coupled electronic states in vertically stacked double *InAs/GaAs* quantum dot molecule

We considered lowest energy states of electrons confined in asymmetrical circular vertically stacked double *InAs/GaAs* quantum dot molecule [see insert (a) in Fig. 6]. The most important difference of this molecule from those usually discussed in literature is that our quantum dots have the same height h, but substantially different radii $r_L > r_U$ (L and U stand for the "lower" and "upper" dots). So, the system is highly asymmetrical in z-direction. To simulate disk-shaped quantum dots we use the effective three-dimensional one-electronic-band Hamiltonian with hard-wall confinement potential (the energy and position-dependent electron effective mass approximation). The external magnetic field **B** is directed along the system axis z.

On the base of this description we demonstrated theoretically a possibility to drive dynamically coupled electronic states (relocate electronic wave functions from one dot to another) by applying external magnetic field. Figure 6 shows the energy dependence on the external magnetic field for three lowest energy states ({1,0,0}, {2,0,0}, and {3,0,0}) of the system. The most remarkable result is anti-crossing between the second ({2,0,0}) and third ({3,0,0}) states (states of the same symmetry) for the system with given parameters. The anti-crossing leads to relocation of the wave functions from one dot to another.

We confirmed this result for multi-electron quantum dot molecules on the based on the current spin density functional theory, a theoretical model of three vertically aligned semiconductor quantum dots. The Kohn-Sham orbitals and energies of six electrons in the molecule with some magnetic fields where computed. It is shown that the six electrons residing in the central dot at zero magnetic field can be changed to such that each dot contains two electrons with some feasible magnetic field (Fig. 7).

This can be potentially interesting in quantum information processing. We pointed out that the model and calculation results presented here can be used as a starting point for further theoretical investigations (including exited states and Zeeman splitting). On the other hand, the main idea to use external magnetic field like a dynamical coupling factor for energy states in highly non-symmetrical nano-systems is more general and potentially very reach.

Publications:

1. O. Voskoboynikov, C.M.J. Wijers, J.L. Liu and C.P. Lee, “Magneto-Optics of Layers of Semiconductor Quantum Dots and Nano-Rings”, to appear in Brazilian Journal of Physics 36, May (2006).
2. O. Voskobyonikov, J. L. Liu, and J. H. Chen, “Magnetically driven coupling of electronic states in quantum dot molecules”, Physica status solidi (c), accepted (2006).
3. C.M.J. Wijers, O. Voskoboynikov, and J.L. Liu, “A hybrid model for the magneto-optics of embedded nano-objects”, Physica status solidi (c), accepted (2006).
4. C.M.J. Wijers and O. Voskoboynikov, “Induction in a Dielectric Sphere: Bulk or Surface”, submitted to American Journal of Physics (2006).
5. C.M.J. Wijers, J-H. Chu, J.L. Liu and O. Voskoboynikov, “The Optical Response of Layers of Embedded Semiconductor Quantum Dots”, submitted to Physical Review B (2006).
6. J. L. Liu, J. H. Chen, O. Voskoboynikov, “A Model for Semiconductor Quantum Dot Molecule Based on the Current Spin Density Functional Theory”, submitted to Computer Physics Communications (2006).
7. O. Voskobyonikov, J. L. Liu, and J. H. Chen, “Magnetically driven coupling of electronic states in quantum dot molecules”, Abstracts of the 4th International Conference on Semiconductor Quantum Dot, France, May (2006).
8. C.M.J. Wijers, O. Voskoboynikov, and J.L. Liu, “A hybrid model for the magneto-optics of embedded nano-objects”, Abstracts of the 4th International Conference on Semiconductor Quantum Dot, France, May (2006).
9. C.M.J. Wijers, “Hybrid Models in Optics: Combining the best from the Discrete and Continuum Worlds”, Talk at Mini-Workshop on Computational Mathematics and Physics, Kaohsiung, 24th February (2006).

Figures:

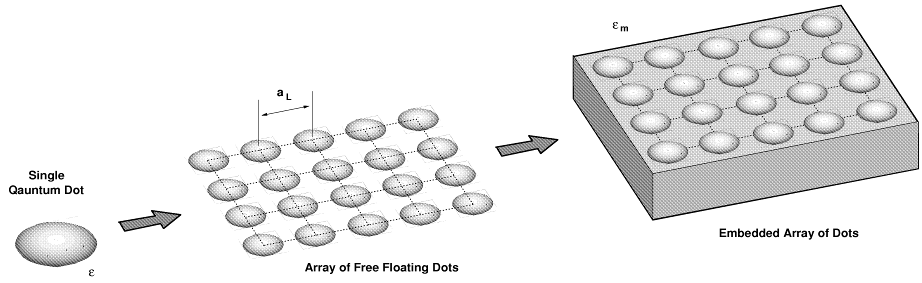

Fig. 1. From a single quantum dot (nano-object) to an array and next to an embedded array of quantum dots.

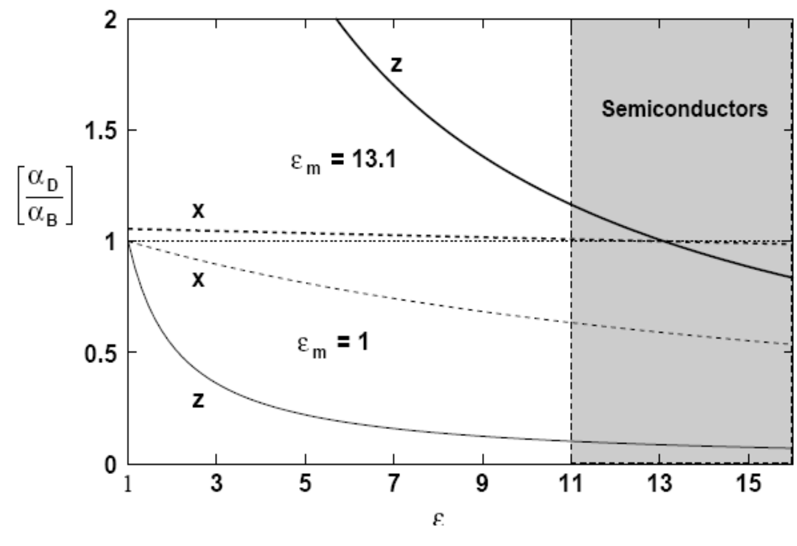

Fig. 2. Influence of embedding upon dressed (α_D) and bare (α_B) polarizability of semiconductor quantum dots for different dielectric media (ε_m).

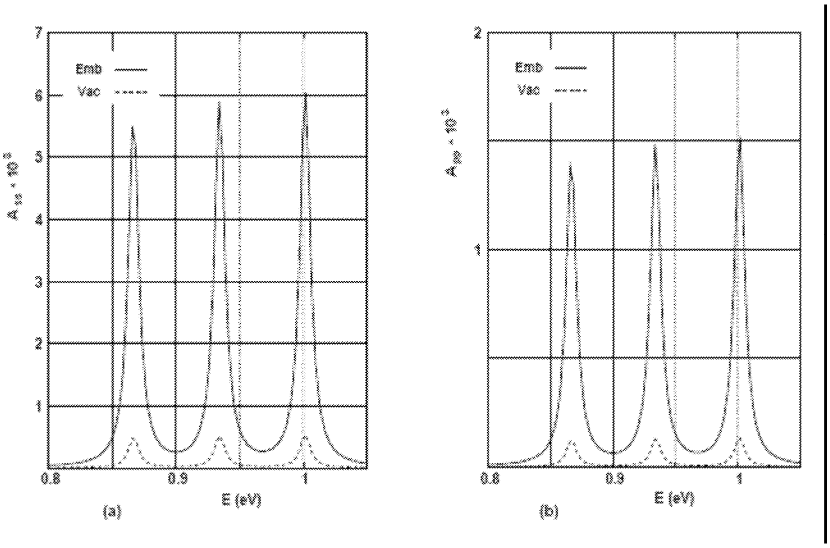

Fig. 3. Influence of embedding ("Emb"- curve) upon optical absorption inside an array of quantum dots. "Vak" stands for the vacuum.

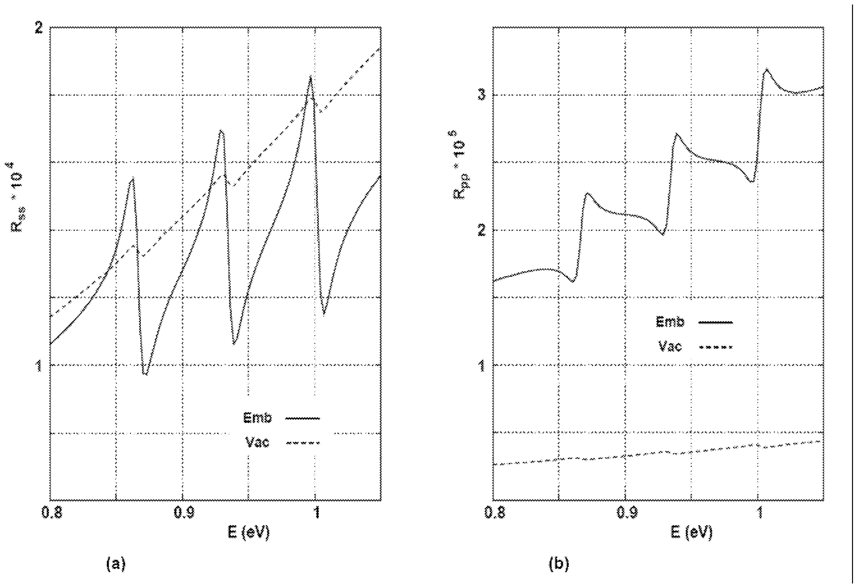

Fig. 4. Influence of embedding upon optical reflectance from an array of quantum dots.

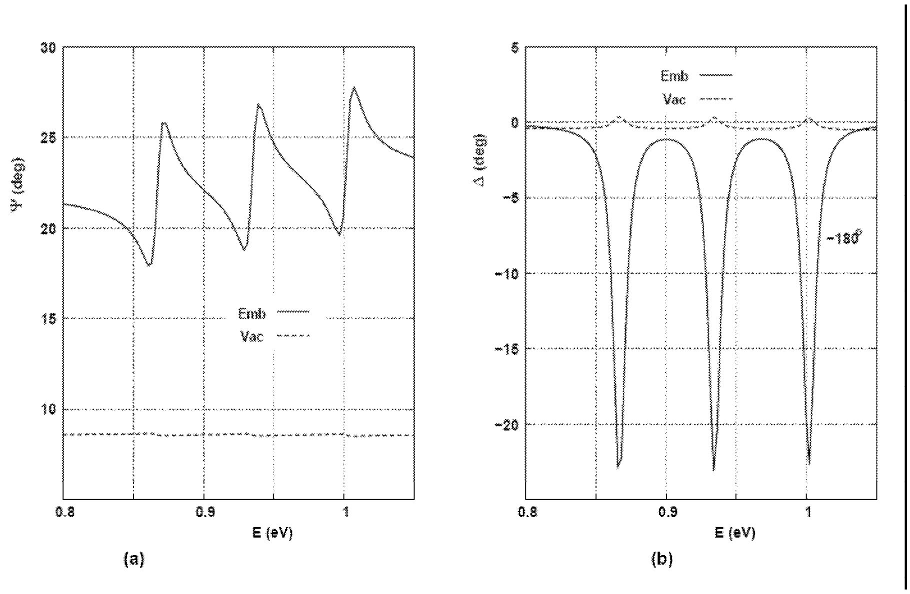

Fig. 5. Influence of embedding upon ellipsometric angles
for an array of quantum dots.

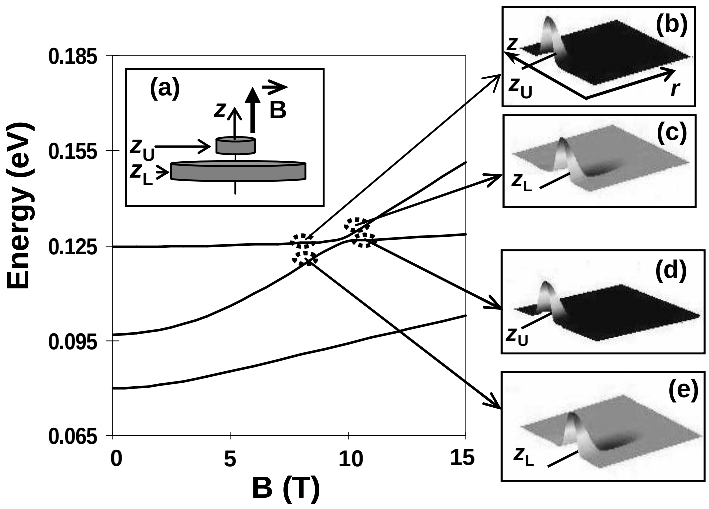

Fig. 6. Asymmetrical double dot molecule in magnetic field:

(a) concept of the system. (b)-(e) locations the wave functions before the level's anti-crossing. (c)-(d) locations the wave functions after the level's anti-crossing.

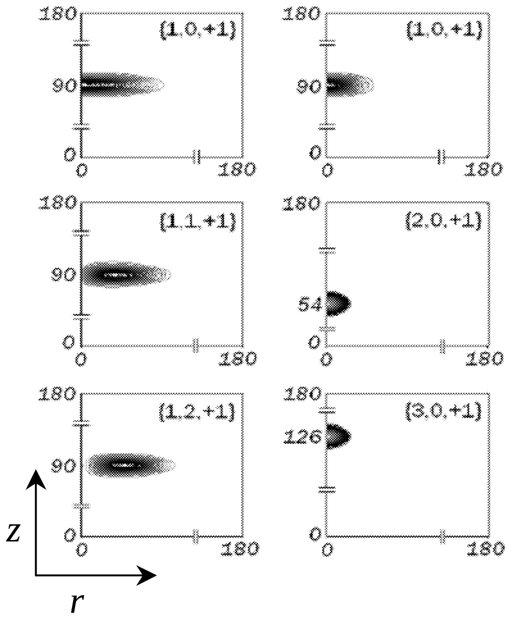

Fig. 7. Contour of Kohn-Sham orbitals {n,l,s} (at z-r plane) at B=0 (left panel) and B=15 (right panel) for six electrons in the three dot molecule.