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A hybrid model for the magneto-optics of embedded nano-objects

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The influence of the surrounding semiconducting matrix upon the polarizability of embedded nano-objects (nano-rings) has been investigated using a hybrid discrete/continuum model. It describes embedded systems by excess discrete dipoles with excess polarizability against a uniform background with the host material dielectric constant. The polarizability combines the static polarizability of an ellipsoidal ring with a dynamic quantum mechanical frequency dependent term. The result of the model for the particular nano-ring host combination investigated is an increased internal reflectance and an overall strong increment of the structure in reflectance/ellipsometric angles, displaying clearly the optical Aharonov-Bohm effect.

1 Introduction

Nano-objects (quantum dots, nano-rings) are nanosized construction elements to compose new types of III-V semiconductor based metamaterials of high potential, particularly in the field of optics. The potential applications range from highly advanced data processing and storage to negative refractive index materials [1]. The use of nanosized elements is necessary to boost the frequency range to the near infrared. The focus in the common modelling of these metamaterials is upon photoluminescence and spontaneous emission, but for e.g. the negative refractive index materials the emphasis has to be upon the basic linear optical properties. In this paper, we want to investigate what happens with the magneto-optical response of nano-rings upon embedding, including the optical Aharonov-Bohm effect. The metamaterial to be investigated consists of a square lattice with lattice parameter a_L, composed of *InAs* nano-rings of characteristic size $a \ll \lambda$ (λ wavelength of light), embedded in *GaAs* as a hostmaterial [2].

2 Theory

We consider nano-rings with dielectric constant ϵ, embedded in a dielectric host material with dielectric constant ϵ_m (see Fig. 1). Flat oblate dielectric ellipsoids will be used for the static response of the nano-rings. The optical response of a single nano-ring should be described in an atomic-like fashion, e.g. by means of Kramers/Heisenberg type of polarizabilities [3]. The hybrid discrete continuum method takes care of the collective electromagnetic response of embedded nano-rings. A proper distinction between the bare polarizability α_B and the dressed polarizability α_D is necessary for that [2]:

$$\mathbf{p} \;=\; \overset{\leftrightarrow}{\alpha}_D \, \mathbf{E}_L \;=\; \overset{\leftrightarrow}{\alpha}_B \left[\mathbf{E}_L + \overset{\leftrightarrow}{\mathbf{t}} \, \mathbf{p} \right] \tag{1}$$

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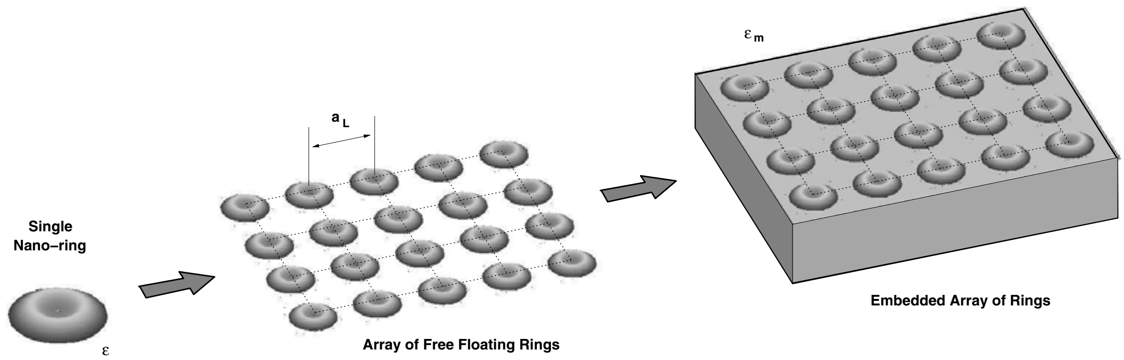

Fig. 1 Conceptual picture of the building of a metamaterial from semiconductor nano-objects (embedded ellipsoidal nano-rings).

where $\mathbf{E}_L$ is the classical local field, which equals the external field $\mathbf{E}_0$ (amplitude E_0) for the case of a single nano-object, $\mathbf{p}$ the dipole strength and $\mathbf{t}$ the intracellular transfer tensor, accounting for electromagnetic selfinteraction. The dressed polarizability α_D is measurable, the bare polarizability α_B follows from theory. We have chosen to add the dynamical contribution $\Delta\alpha(\omega)$, as derived before in [2], to the bare polarizability α_{BE}:

$$\alpha_{BE}(\omega) \;=\; \alpha_{BE} + \Delta\alpha(\omega) \;=\; \epsilon_0 V (\epsilon - \epsilon_m) + \Delta\alpha(\omega)$$

$$\Delta\alpha(\omega) \;=\; \frac{3}{4}\,\frac{e^2}{\hbar}\, r_{eh}^2 \left[\hat{\mathbf{x}}\hat{\mathbf{x}}^T + \hat{\mathbf{y}}\hat{\mathbf{y}}^T\right] \sum_{l=0}^{-2} |\langle F_{hl}|F_{el}\rangle_V|^2\, f_{hl,el}(\omega) \qquad (2)$$

in agreement with [4] and [5]. The embedded bare polarizability α_{BE} was taken from the dressed one α_{DE} using (1). For this dressed polarizability we had to solve the potential $\Phi(\mathbf{r})$ from the Poisson equation, using the same ellipsoidal ring as in [2] with $\zeta = c/a$, oblate elliptic coordinates ξ, η, ϕ and $f = \sqrt{a^2 - c^2}$. Because of symmetry we can use the Ansatz:

$$\Phi_v(\xi, \eta, \phi) \;=\; -E_0 f \sin\eta \left[A_v \sinh\xi + B_v \left(1 - \sinh\xi\ \tan^{-1}\left(\frac{1}{\sinh\xi}\right)\right)\right] \qquad (3)$$

where $v = I$ refers to inner and $v = O$ to outer region. From physics considerations we find that $B_I = 0$ and $A_O = 1$. The coefficients A_I, B_O follow from the boundary conditions for the dielectric displacement $\mathbf{D}$ and electric field $\mathbf{E}$ across the surface. As a result we obtain the excess *dressed* polarizability α:

$$\alpha_{Du} \;=\; \frac{V(P - P_m)}{E_0} \;=\; \epsilon_0 V \left[\frac{\epsilon_m(\epsilon - \epsilon_m)}{\epsilon_m + N_u(\epsilon - \epsilon_m)}\right]$$

$$N_z \;=\; \frac{1}{1 - \zeta^2}\left(1 - \frac{\zeta\, \cos^{-1}\zeta}{\sqrt{1 - \zeta^2}}\right) \qquad (4)$$

with $u = x, y, z$. $V = \frac{4}{3}\pi a^2 c$ is the ellipsoid volume and P, P_m ring, host polarization density. The other orientations are found by using $N_{x,y} = (1 - N_z)/2$. We approximate the external electric field by electric dipole fields. For a system of embedded nano-objects we have to solve the system of equations:

$$\overset{\leftrightarrow}{\alpha}{}^{-1}_{BEi}\, \mathbf{p}_i - \frac{1}{\epsilon_m} \sum_{i \neq j} \overset{\leftrightarrow}{\mathbf{t}}_{ij}\, \mathbf{p}_j \;=\; \mathbf{E}_0 \qquad (5)$$

where $\mathbf{t}_{ij}$ is the frequency dependent vacuum intercellular transfer tensor, screened by ϵ_m, and α_{BEi} is the $\alpha_{BE}(\omega)$ from (2). The optical response of an embedded square lattice of nano-objects can be calculated using the (Vlieger) expressions [6] for $r_{ss}(A_y, f_k, \theta_i)$, $r_{pp}(A_x, A_z, f_k, \theta_i)$ for the reflected electric fields from a square lattice with lattice constant a_L, as used before in [2]. The key parameters in these expressions, being A_u, k_m, are the only elements which change upon embedding:

$$A_u = \alpha_0\, \alpha_{BEu}(\omega)^{-1} - \frac{1}{\epsilon_m}\,(\mathrm{f}'_u + \alpha_0\, t_u)$$

$$f_k = 2\pi i a_L \sqrt{\epsilon_m}\,\frac{\omega}{c} \qquad t_u = -\frac{N_u}{\epsilon_0\, V} + \frac{ik^3}{6\pi\epsilon_0} \tag{6}$$

where $\alpha_0 = 4\pi\epsilon_0 a_L^3$. The planar transfer tensor $\mathbf{f}$ is made dimensionless through $\mathrm{f} = \alpha_0\, f$ and gets the fixed values given in [2]. In (6) $\mathbf{t}$ is the intracellular tensor for the vacuum situation. With the description above the entire theoretical derivation makes only use of bare polarizabilities. During the calculations we will use the center-hole ellipsoid described in [2].

3 Numerical results

We show the results of the influence of embedding upon the optical response of an embedded square lattice of nano-rings. We use the same parameters, apart from $\epsilon = 15.15, \epsilon_m = 13.1$, as used in [2]. We find a static bare embedded polarizability $\alpha_{BE} = 6.21650 * 10^{-4}\ \alpha_0$ and a static vacuum bare polarizability $\alpha_{BV} = 4.23042 * 10^{-3}\ \alpha_0$. So the bare polarizability drops by a factor of 0.147 upon embedding. The static anisotropy, the ratio α_x/α_z, drops for the dressed polarizabilities from 7.12 for vacuum to 1.13 for embedded. This is because the dressed polarizability decreases for the x, y direction and increases for the

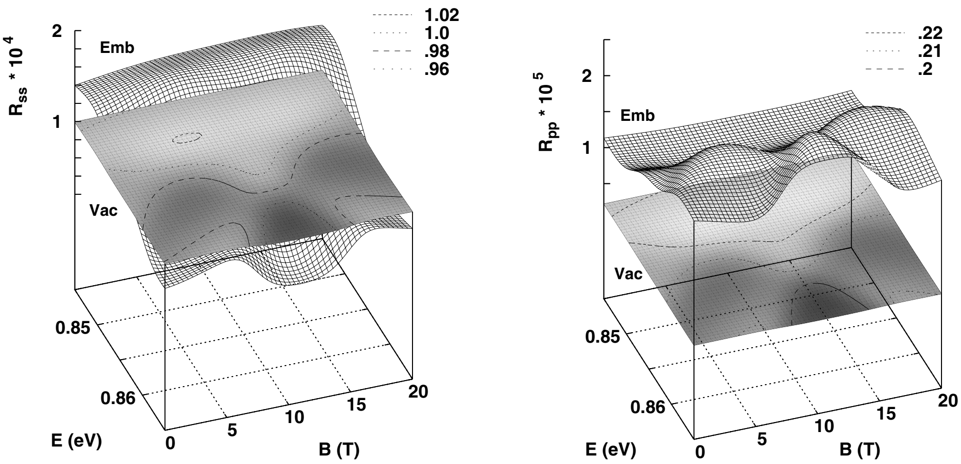

Fig. 2 Reflectance R for angle of incidence $\theta_i = 60°$. Left: R_{ss}, right: R_{pp}. Dashed curves: vacuum (no embedding), Solid curves: embedding with $\epsilon_m = 13.1$

z-direction. Screening is the mechanism responsible for all these phenomena.

For the angle of incidence $\theta_i = 60°$, close to the Brewster angle, the reflectance's for the two polarization directions s and p are shown in Fig. 2. The left panel shows that there is only weakly decreased reflectance for the s-component upon embedding. For the p-component the embedded reflectance is larger than the vacuum reflectance up to a factor of 3. The structure is due to the dynamical quantum mechanical part of the polarizability $\Delta\alpha(\omega)$ and is much stronger for embedded than for vacuum.

The ellipsometric angles Ψ and Δ, representing experimental values [2], are relative quantities, not dependent upon the absolute reflected intensities. For the ellipsometric angle Ψ the vacuum results are

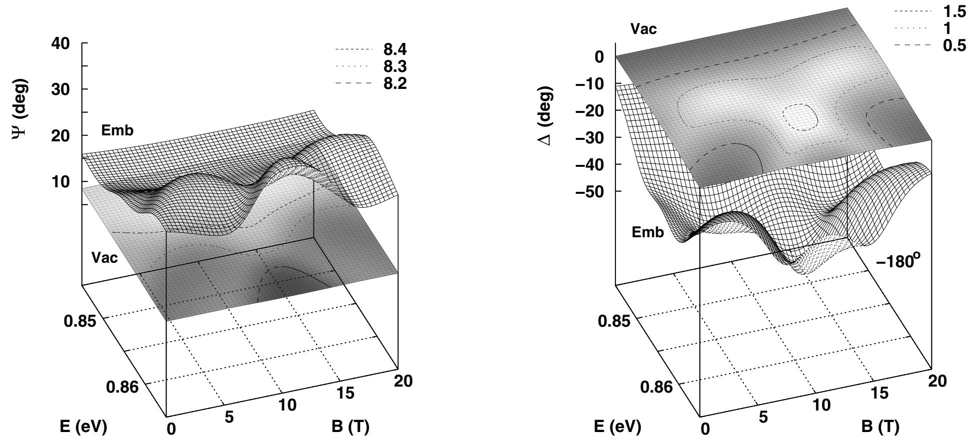

Fig. 3 Ellipsometric angles Ψ, Δ for angle of incidence $\theta_i = 60°$. Left: $\Psi(°)$, right: Vacuum: $\Delta(°)$, embedded: $\Delta(°) - 180°$. Dashed curves: vacuum (no embedding), Solid curves: embedding with $\epsilon_m = 13.1$

systematically below the embedded results (Fig. 3). The variation in Ψ increases from about $0.25°$ to $13°$ upon embedding at $E = 0.865\ eV$. For the embedded case the mean value of Ψ centers now around $30.5°$ there. We see that the vacuum and embedded values for Δ are about $180°$ out of phase. The absolute overall variation in Δ increases from $1.7°$ to $42°$ upon embedding. The variation in Ψ, Δ reflects the optical AB-effect and is comfortably within range of an ellipsometer.

4 Summary and conclusions

We have modelled the optical response of a square lattice of nano-rings by means of a hybrid discrete-continuum model, using excess dipoles against a uniform background with the dielectric constant of the host material. Dielectric oblate ellipsoids are used to model the static response of the ellipsoidal ring. In this model the excess polarizability of the ring can be larger than the vacuum polarizability. All electromagnetic interactions in the system are screened by the dielectric constant of the host material. The dynamical quantum mechanical contributions responsible for both the magnetic field and the frequency dependence are added to the embedded bare polarizability. Embedding increases the reflectance (upto a factor of 3). The structure in the reflectance and the ellipsometric angles increases from measurable (a few tenth of a degree) to large (upto 50 degree). These enhancements caused by embedding are very favorable to measure the optical Aharonov-Bohm effect.

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