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ELASTIC FIELDS OF SURFACE QUANTUM DOTS

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ABSTRACT

The elastic fields of three-dimensional quantum dots, and the interaction energy between them, are determined by finite element analysis. The results from the analysis are then used in optimization of several cases of multiple dot ordering on the surface of a semiconductor. The strain energy in the model remains constant, when a certain plateau has been reached, even though dot height is increased. Furthermore, for a range of idealized geometries, the shape of the quantum dot has little impact on the strain energy, and thereby the interaction energy.

INTRODUCTION

The focus of this research project is to determine the elastic stress fields of three-dimensional self-assembled quantum dots (SAQDs) and the elastic interaction energy between them. In particular, the effect of interaction energy on the spatial ordering of quantum dots is investigated.

Both for understanding ordering, as well as the subsequent effects on electronic properties in SAQD structures, several classes of theoretical models have evolved. Romanov et al. [1] considered the elastic fields of quantum dots in subsurface layers. Their work has then been extended to surface quantum dots [2].

In the present study, the purpose is two-fold: firstly, to determine the elastic fields in 3D quantum dots and the surrounding substrate, by means of finite element analysis, in order to assess the effect of lattice mismatch, dot volume, and dot/surface contact area on the induced stress fields and elastic energy. Secondly, to investigate the elastic interaction between quantum dots and the impact of the separation distance between the dots on the interaction energy. The results are used to establish an interaction law, that is, interaction energy versus separation distance. The interaction law is then used to study ordering of multiple quantum dots on the surface of a semiconductor. The study is carried out for several simple quantum dot shapes, such as pyramids, cylinders and spherical caps. Ordering of multiple identical dots is optimized using an ES(1+1)-algorithm for the cases of periodic dispersion of dot material and dispersion of fixed volume of dot material.

ELASTIC SOLUTIONS FOR AN ISOLATED QUANTUM DOT

SADQ formation is commonly observed in large mismatch epitaxy of chemically similar materials, for example, [3]. If a dot with lattice parameter a_d is deposited on the surface of substrate with lattice parameter a_s, the misfit strain ε_m is taken as $(a_s - a_d)/a_d$. The effect of the lattice mismatch in the finite element models was achieved via effective thermal expansion of the quantum dot material $\varepsilon_m = \triangle\alpha\triangle T$ where $\triangle\alpha$ and $\triangle T$ is the difference between the substrate and the quantum dot of the coefficient of thermal expansion and temperature respectively. The mismatch strain was taken as unity. For simplicity, the material properties chosen were shear modulus $\mu = 1$, Poisson's ratio $\nu = 0.3$ and hence Young's modulus $E = 2.6$

By computing the total strain energy in the FE-model, it is observed that the strain energy increases with increased volume of the quantum dot until it attains a certain height. At that plateau, the strain energy remains constant even though dot height is increased.

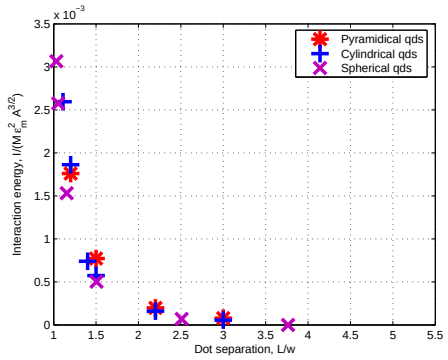

Figure 1. TOTAL NORMALIZED STRAIN ENERGY AS A FUNCTION OF ASPECT RATIO, WHERE THE ELASTIC MODULUS IS $M = E/(1-v)$, L: DOT SEPARATION, I: INTERACTION ENERGY, w: BASE WIDTH OF DOT AND A: DOT/SUBSTRATE CONTACT AREA.

INTERACTION BETWEEN QUANTUM DOTS

Interaction energy is the extra energy needed to create a quantum dot in a certain place when another dot already exists nearby, over and above the energy that is required to create the dot when it is isolated. For quantum dots of fixed shape and size, interaction varies only with the distance separating the dots, providing no external interference. The interaction energy is calculated by $I = TS_L - TS_\infty$ where TS_L is the total strain energy for a given distance L, between the centers of the dot bases, and TS_∞ is the total strain energy when L is so large that no interaction exists.

Figure 1 shows the normalized interaction energy as a function of dot separation distance. All dot shapes tested, i.e., pyramidical, cylindrical and spherical, give results on the same interaction curve. This shows, at least for the cases tested, that the interaction energy of SAQDs is fairly independent of dot shape.

ORDERING OF MULTIPLE QUANTUM DOTS ON THE SURFACE OF A SEMICONDUCTOR

Dot ordering is important in practise. For example, the fabrication of quantum dot laser, depends on a dense array of quantum dots, uniform in size and shape [4].

Three types of pyramidical dots are used, with aspect ratios $AR = h/b = 1$ (type 1), 1/2 (type 2) and 1/3 (type 3), all equal in height, where h is the height of the dot and b is the base width. Interaction energy was plotted, with results from FEM-calculations, as a function of dot separation for all dot types. Each curve was then fitted with an appropriate equation which from then on was used as a substitute for the FEM to calculate the interaction energy.

The total interaction energy in a system of multiple quantum dots was calculated by

$$I_{total} = \frac{1}{2} \sum_{\substack{i=1 \\ i \neq j}}^{N} \sum_{\substack{j=1 \\ i \neq j}}^{N} I_{ij}^{k \leftrightarrow m} \tag{1}$$

where N: total number of dots, I_{ij}: interaction energy between dots i and j, $k \leftrightarrow m$: dot types where k and m are types 1, 2 or 3. The 1/2 in Eqn. 1 is there to avoid recount, since eg $I_{12}^{2\leftrightarrow 3} = I_{21}^{2\leftrightarrow 3}$. The equation is then used in the ES(1+1) optimization code, as the fitness function, to position the quantum dots at locations which minimize the total interaction energy. When using this method to find the optimal positions for two, four and five dots on the surface of the semiconductor, each results in the same ordering as on an ordinary dice for the number in question. Then identical dots were fixed at the corner points of an equilateral triangle, square, pentagon and hexagon. In all cases there is a point of stable equilibrium at the center of area. Point of stable equilibrium is a point where the dot has no tendency to move to another location since it is already at a point of lower interaction energy than its nearest neighborhood. This is valid for an equilateral n-polygon when n = 3, 4, 5 and 6, and can thus be assumed to apply for all n $>$ 2 when the dots are identical. Dispersing fixed volume of dot material over the surface of the substrate, in all cases tested, showed that two large dots are energetically a more feasible solution than multiple smaller dots.

CONCLUSIONS

This study resulted in several conclusions, some of which are intuitively understood but others give insight into areas which are more involved. For example increasing the height of a quantum dot only increases the strain energy up to a certain height. When that plateau has been reached the strain energy in the model remains constant even though dot height is increased. If discarding size effects, the shape of the quantum dot has little impact on the strain- and interaction energy in the models.

REFERENCES

[1] Romanov, A. E., Beltz, G. E., Fischer, W. T., Petroff, P. M., and Speck, J., 2001. "Elastic fields of quantum dots in subsurface layers". *J. of Appl. Phys.*, pp. 4523–4531.

[2] Beltz, G. E., Jonsdottir, F., Chin, K. A., Romanov, A. E., and Speck, J. S., 2005. "Simple description of the elastic fields of coherent surface islands". *submitted to Appl. Phys. Lett.*

[3] Eaglesham, D. J., and Cerullo, M., 1990. "Dislocation-free stranski-krastanov growth of ge on si(100)". *Phys. Rev. Lett.*, **64**, pp. 1943–1946.

[4] Borovitskaya, E., and Shur, M. S., eds., 2002. *Quantum Dots: Selected Topics in Electronics and Systems*, Vol. 25. World Scientific.