第26卷 第7期 半 导 体 学 报 Vol. 26 No. 7
2005年7月 CHINESE JOURNAL OF SEMICONDUCTORS July, 2005

Elastic Strain Field Distribution of a Self-Organized Growth Lensed-Shaped Quantum Dot by Finite Element Method*

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Abstract: The stress and strain fields in self-organized growth coherent quantum dots (QD) structures are investigated in detail by two-dimension and three-dimension finite element analyses for lensed-shaped QDs. The nonobjective isolate quantum dot system is used. The calculated results can be directly used to evaluate the conductive band and valence band confinement potential and strain introduced by the effective mass of the charge carriers in strain QD.

Key words: quantum dot; elastic strain field; stress

PACC: 0365; 2110D; 7280E

CLC number: O469 **Document code:** A **Article ID:** 0253-4177(2005)07-1317-06

1 Introduction

Quantum dots have drawn great interest due to their potential in the fabrication of a wide variety of novel photoelectric and microelectronic devices, such as a light emitting diode (LED), solar cell, semiconductor quantum dot laser, and single electron transistor[1,2]. As it is well known, the strain, which originates from the lattice mismatch between the quantum dot and the substrate material, is the driving force of the self-organize growth style. Recent studies also show that the misfit strain has a great effect on the electronic structure of the produced three-dimension (3D) quantum island in the Stranski-Krastanow (S-K) growth. Therefore, the elastic field in and around the QDs should be studied to give a good evaluation of the electronic structure and the performance of quantum dot devices. In this paper, we give detailed descriptions of the elastic field of the lensed-shaped quantum dot.

2 Model building

The modeling of a strain due to lattice mismatch is straightforward, so long as the lattice remains coherent (the strain is not relaxed by dislocation). In this condition, strain calculation can be made by either a continuum elasticity (CE) approximation or an atomic elasticity (AE) named valence force field method. CE approximation calculations are usually made with commercial finite-element software, such as ANSYS. The atomic level models are computationally more intensive and limited to small systems, while CE calculation is

* Project supported by the State Key Program for Basic Research of China (No. 2003CB314901), the National High Technology Research and Development Program of China (No. 2003AA311070), and the Open Project of State Key Laboratory on Integrated Optoelectronics

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Received 25 September 2004, revised manuscript received 22 February 2005

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fast and adept at multiple quantum dot systems modeling. The strain results agree well except at the edges of the structure, so the calculated band structure modifications based on both methods are small. In this paper, the CE calculation method is adopted to analyze the strain field of the lensed-shaped QD. For simplicity, the flowing simplifications are used:

(1) a two-dimension axis-symmetrical model;

(2) an isolated QD, which ignores the elastic interactions among the multiple QDs;

(3) the anisotropy characteristics of the material, either the QD or the matrix material, are ignored and we assume there are identical isotropic elastic coefficients.

The lensed-shaped quantum dots can be found in Ref. [5]. Figure 1 shows a schematic cross-sectional view of an isolated QD. The QD is grown along the (001) direction. As the calculations are carried out with axial symmetry, all results will be displayed for $y = 0$. In Fig. 1, the highest value of the quantum dot defined as from the top of the wetting-layer to the top of the quantum dot is 5nm, the thickness of the capper layer is 11nm defined from the substrate to the top of the model, the thickness of the substrate is 30nm and the lateral length of the substrate is 50nm.

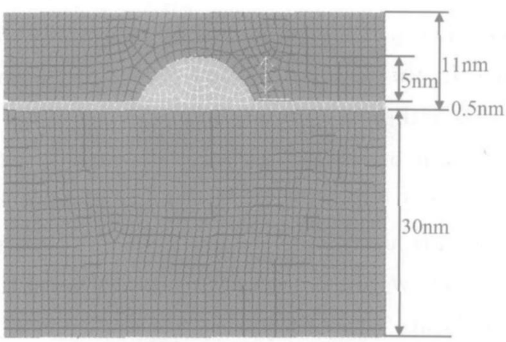

Fig. 1 Schematic of the two-dimension lens shaped isolated quantum dot, which have been meshed by ANSYS

In our axi-symmetric model systems, the substrate, wetting-layer, the quantum dot, and the cap layer are built separately. We use the command "Glue" of the ANSYS to merge them together and form the shapes, as shown in Fig. 1. We treat the whole system as a super cell. To solve the problem, we apply displacement boundary conditions to the system. The boundary conditions consist of the following: for the lateral surface, the displacement is fixed along the normal direction of the surface; the bottom surface is the substrate material and the displacement is fixed in all degree; the top surface is free in all degrees. In Fig. 1, the origin of the coordinate system is located at the left-bottom corner. The growth direction is along the [001] direction pointing upwards, which means the QD is growing on the (001) surface. In discussions about the tow-dimensional model, we do not discuss the specified material, and we prescribe the Yong' modulus and Poisson rate, which are $E = 86$GPa and $v = 0.3$, respectively. For the whole cell, the mismatch strain is $\varepsilon_0 = a_s - a_{QD} / a_{QD} = -0.04$, where a_s and a_{QD} are the lattice parameters of the substrate and the QD material. To model the lattice mismatch that is responsible for the island formation, a pseudo thermal expansion of the island and the wetting-layer is applied and thus makes each section of the material experience a uniform thermal expansion in all directions. The temperature is raised by 1K and the material thermal expansion coefficient is $|\varepsilon_0| = 0.04$. Thus, the thermal strain is defined as $\varepsilon_T = \varepsilon_0 \Delta T$ and no other load is applied to the super cell.

Although the two-dimensional axi-symmetric model is sufficient to give us an insight into strain distribution, it reflects only one plane. The two-dimensional plane is equivalent to the $y = 0$ plane in the three-dimension model. As an example, we give the GaAs quantum dot growth on the InAs substrate along the (001) direction. The schematics are shown in Fig. 2, where we use the three-dimensional model and only the cap layer and the quantum dot-wetting layer are shown. The size of the system is shown in Fig. 1 and the material characteristic parameters are shown in Table 1. An advantage of the three-dimensional model is that it gives a more complete picture of the strain distribution of self-organized quantum dot systems ,since the strain distribution of any arbitrary plane can be easily obtained.

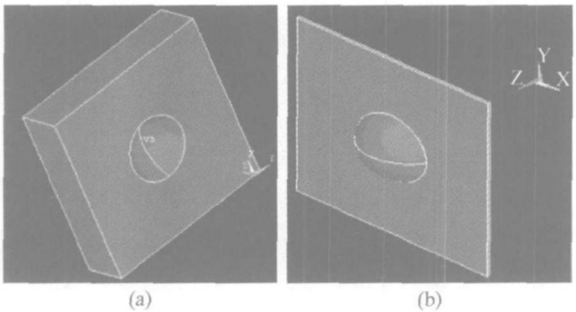

Fig. 2　Schematic of three-dimension lens isolated quantum dot　(a) Cap layer ; (b) The quantum dot and wetting-layer

Table 1　Isotropic properties of GaAs and InAs

Material	E/ GPa	v	Lattice/ nm
GaAs	86.96	0.31	0.565325
InAs	51.42	0.35	0.605830

3　Results and discussion

The analysis model is a structure static mechanics model ,in which we adopt the PLANE 183 as the element model. Figures 3 (a) and (b) give the strain distribution in the super cell of the strain component of ε_{xx} and ε_{zz} . From Fig. 3 (a) we can see the maximum of the ε_{xx} strain is located near the top of the quantum dot , while the strain near the wetting-layer is small compared with the area above the QD. The strain component of ε_{zz} is opposite of the strain distribution of ε_{xx} ,with the minimum position located on top of the QD and the maximum area distributed around the QD that contacts with the wetting-layer. Figures 4 (a) and (b) show the stress distribution , which are approximately with the strain distribution. The strain and stress penetrate into the substrate about the height of about one or two times the QD height. Figure 5 gives the strain distribution of the QD along the central line form the bottom of the substrate to the top of the cap layer. We can see there is a big strain value in the quantum dot region. However , the

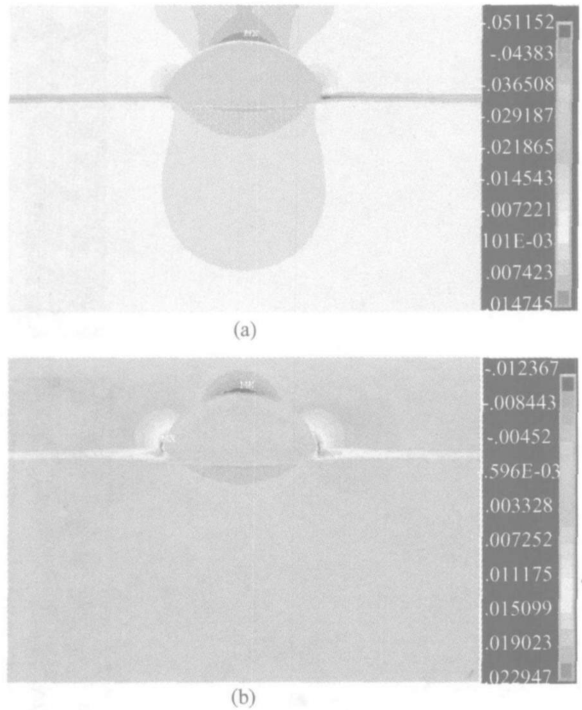

Fig. 3　Contour plots of strain distribution of the two-dimension axi-symmetri super cell in the components of ε_{xx} (a) and ε_{zz} (b)　The maximum and minimum values are indicated in each plot respectively.

strain variation in this region is small enough that one can think it is a uniform strain in either ε_{xx} or ε_{zz} components. There is a great variation of the strain in both the interface of the quantum dot with the substrate and the quantum dot with the cap layer. With the depth increasing along the substrate direction , the strain is gradually reduced to zero ,as shown in Fig. 5. The ε_{xx} component in the quantum dot experiences a compression strain , while in the cap layer and the substrate the material experiences a tensile strain.

The hydrostatic strain is very important to the conduct band confinement potential[4]. In Fig. 6 , the hydrostatic strain along the central axis is presented. As can be seen , the confinement in the substrate and cap layer is a very small value and can be approximated as zero ,while in the quantum dot the hydrostatic strain is just like a potential well. Thus the whole effect of the hydrostatic to the quantum dot in the (001) direction is just like a finite depth potential well.

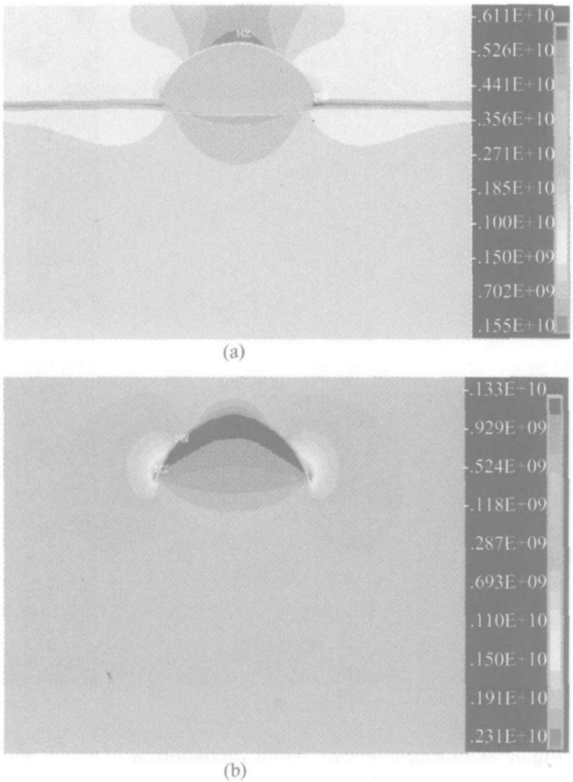

Fig. 4 Contour plots of stress distribution in the two-dimension axi-symmetric super cell in the components of σ_{xx} (a) and σ_{zz} (b) The maximum and minimum value are indicated in each plot respectively.

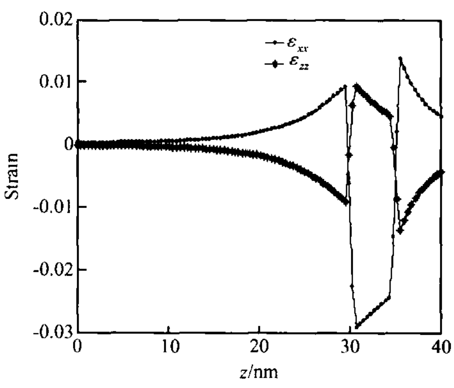

Fig. 5 Strain of ε_{xx} and ε_{zz} distribution through the center line of the quantum dot from the bottom of the substrate to the top surface of the cap layer

For the three-dimensional InAs/ GaAs/ quantum dot system, the lattice mismatch is - 6.7 %. The calculation of the three-dimensional model is very time-consuming; however, using the three-dimension model, we can analyze the stress or strain distribution in any arbitrary plane. In Fig. 7 we

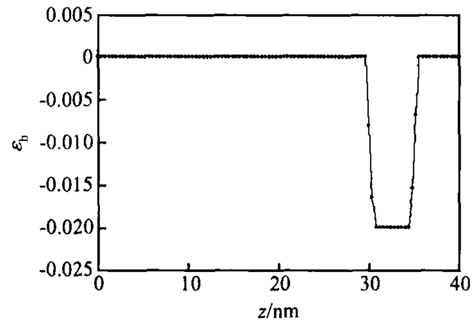

Fig. 6 Hydrostatic strain along the center line of the quantum dot from the bottom of the substrate to the top surface of the cap layer

show the ε_{xx} strain distribution in the z plane, which is about 6nm distance from the top of the quantum dot. The tensile strain areas are located just above the top of the quantum dot and the

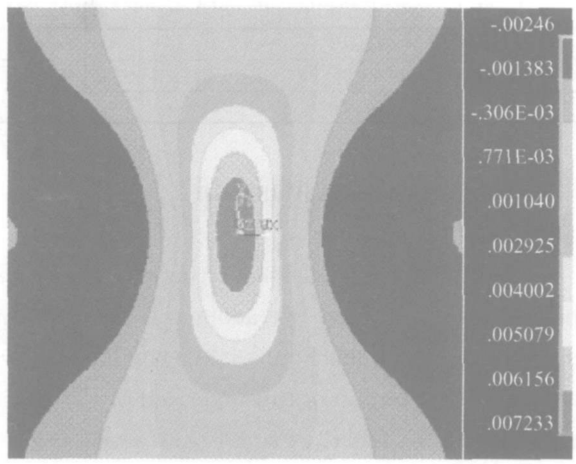

Fig. 7 ε_{xx} strain contour plots in $z = 11$ plane in the three-dimension model of GaAs/ InAs quantum dot system where the distance of the plane to the top of quantum dot is 6nm

strain decreases gradually in the plane. The other strain components in the plane are shown in Fig. 7. The strain distribution in the top surface plane [001] is very important, because in the S-K growth model the continuous growth vertical ordering is strongly influenced by the strain energy density in the second wetting-layer. Generally, nuclei are easy to form in the location of an energy minimum. In Fig. 8, we show the ε_{yy} and ε_{xy} strain profile in the whole three-dimensional model. For the three-dimensional strain ε_{yy} distribution, there is a symmetrical-plane of $y = 0$,while for the ε_{xy} strain ,there is no symmetrical-plane but the strain is still somewhat symmetrical and the strain value is opposite beside the $x = 0$ plane. The ε_{xy} is almost twice as small as the ε_{yy} in most parts of the system ,excluding the part near to the interface of the quantum and matrix material.

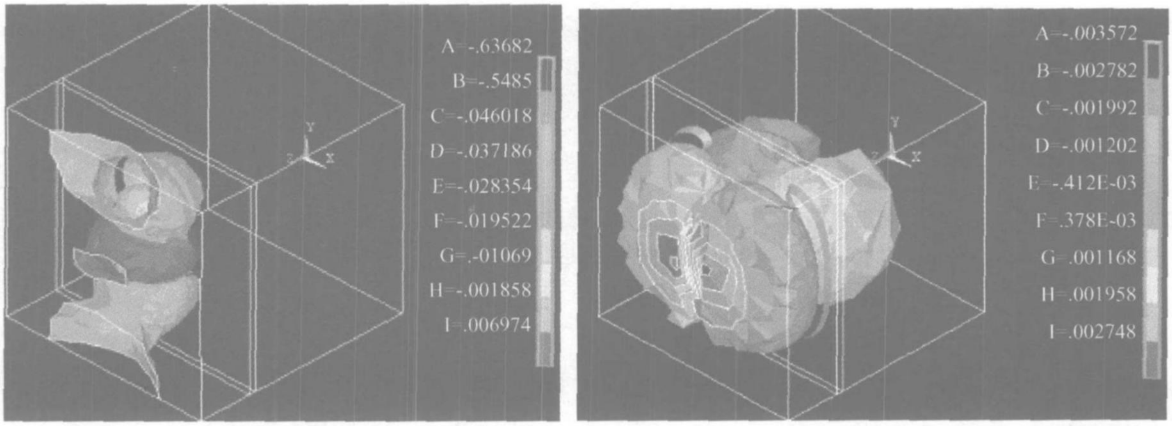

Fig. 8　ε_{yy} and ε_{xy} strain contour profile in the three-dimension model of GaAs/ InAs quantum dot system

4　Conclusion

The hetero quantum dot system is analyzed using two-dimensional axi-symmetrical models in a general form. Although the model is simplified greatly and the shape of the quantum dot is not always a regular lens shape ,as discussed above ,our simulation in the system can easily be extended to complex shaped quantum dots. As an example ,in the GaAs/ InAs quantum dot system we use the three-dimensional model. This model can not only give similar results to the axi-symmetrical models , but also gives the strain distribution in the whole system in the style of an equal-vale plane ,as shown in Fig. 8. In this form ,we can see more information about the strain in the inner part of the system. Detailed strain information in the other arbitrary plane can easily be obtained by cutting the three-dimensional system ,as the calculation of the three-dimensional model is very time consuming.

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有限元法分析透镜形自组织生长量子点的弹性应变场分布*

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摘要: 利用有限元法对应变自组织生长量子点的应力应变分布进行了系统分析. 给出了抽象的孤立量子点系统模型,采用有限元分析方法,利用二维和三维模型对透镜形的量子点内部及周围材料的应力应变进行了计算,计算结果可以直接应用于量子点应变场对导带和价带限制势以及载流子有效质量的影响,从而用于精确计算量子点的电子结构.

关键词: 量子点; 弹性应力场; 应力
PACC: 0365; 2110D; 7280E
中图分类号: O469 **文献标识码**: A **文章编号**: 0253-4177(2005)07-1317-06

* 国家重点基础研究发展计划(批准号:2003CB314901),国家高技术研究发展计划(批准号:2003AA311070)和集成光电子学国家重点联合实验室开放课题资助项目

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2004-09-25 收到,2005-02-22 定稿 ©2005 中国电子学会