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Periodically Grown Quantum Nanostructures with Arbitrary Geometries: Periodicity Effects on the Induced Electro-Elastic Fields

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Abstract

Quantum nanostructures (QNSs), due to their widespread and attractive physical, optical, and electronic properties, have been at the center of attention of many nanoscience and nanotechnology researches. In order to predict the electro-mechanical behavior of QNSs, accurate determination of the electro-elastic fields induced by quantum wells (QWs), quantum wires (QWRs), and quantum dots (QDs) in such nanostructures would be of great importance and particular interest. In this study, by utilization of the electro-mechanical eigenfield concept in conjunction with the Fourier series technique, an analytical solution is presented which gives the electro-elastic fields induced by one-, two-, and three-dimensional periodic distribution of QWs, QWRs, and QDs, respectively. This methodology takes into account the electro-mechanical couplings of elastic and electric fields within the piezoelectric barrier as well as the interaction between periodically grown QWRs and QDs. The latter would be so important since the density of the periodically grown QNSs will have significant effects on the induced electro-elastic fields within both the QNSs and the surrounding barrier; this issue is addressed precisely in the present study by measuring the induced electro-elastic fields due to different periodicities of pyramidal QDs. Furthermore, the current formulation is capable of treating arbitrary geometries of QWRs and QDs which makes the solution more interesting and powerful.

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Keywords: quantum nanostructures; quantum dots; quantum wires; quantum wells; electro-elastic fields

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1. Introduction

As the applications of quantum nanostructures (QNSs) have been considerably increased in recent decades due to their interesting optical and physical specifications, these nanostructures have attracted the attention of lots of scientific and technological researches in various fields. QNSs including quantum wells (QWs), quantum wires (QWRs), and quantum dots (QDs) have been widely utilized in microelectronic devices especially in light emitting diodes (LEDs), laser diodes, solar cells, and memory capacitors. Furthermore, interesting properties of QNSs have made them so valuable for bioengineering and biomedical applications especially in labeling and tracking cells and genes for cancer diagnosis among many different applications. In studying and utilization of QNSs for many of the mentioned applications, determination of their electro-mechanical behavior as well as their internal electro-elastic fields is of particular interest, rundmann et al. (1995); Bimberg et al. (1999). The internal electro-elastic fields within QNSs arises from the initial lattice mismatch between QWs/QWR/QDs and their surrounding barrier, Singh (1993). This initial lattice mismatch induces elastic fields as well as electric fields within both the QNSs and the piezoelectric barrier.

The electro-elastic fields of QNSs have been investigated by many researchers in recent years. For instance, the analytic forms for the elastic fields of a single spherical QD within a purely elastic and isotropic medium have been proposed by Grundmann et al. (1995); they have also studied the more complicated case of a single pyramidal QD by employing finite element analysis. Faux and Pearson (2000) based on an expansion of the strain Green's tensor, provided an analysis for QDs within anisotropic elastic media. Shodja and Rashidinejad (2014) presented analytical formulations for accurate determination of the electro-elastic fields of interacting functionally graded QNSs with arbitrary shapes and general anisotropy within piezoelectric media. The interaction between QWs/QWRs/QDs is an important issue in determination of the induced electro-elastic fields since QNSs are usually grown with high densities and periodic distributions to enhance their performance. Periodically grown QNSs have been observed by many researchers via transmission electron microscopy (TEM) images, Bimberg et al. (1999); Xu et al. (2007).

The interaction effects of periodically grown QNSs and especially QD structures with different periodicities within a piezoelectric barrier have not been studied yet. In this paper, an analytical methodology pertinent to determination of the induced electro-elastic fields of periodically grown QNSs is given and subsequently, effects of the distance of QNSs and their periodicities on the induced piezoelectric fields are studied and explained. For this reason, periodically grown pyramidal QDs which are the most common geometry between many possible shapes of QDs, have been considered and the effects of their distribution periodicity on the induced strain field have been accurately determined and illustrated. The results show that the induced fields may be remarkably affected when the period of the distribution become shorter and the adjacent QDs become closer to each other.

2. Periodic distribution of quantum nanostructures

Quantum nanostructures (QNSs) with one-, two-, and three-dimensional confinements known, respectively, as quantum wells (QWs), quantum wires (QWRs), and quantum dots (QDs) induce both elastic and electric fields within themselves and the surrounding piezoelectric barrier. These electro elastic fields arise due to the lattice mismatch between the QNSs and the piezoelectric barrier. The lattice mismatch of QNSs grown within a piezoelectric barrier is usually modeled as an initial strain field within the QNSs as described by Bimberg et al. (1999) and Shodja and Rashidinejad (2014). Initial misfit strains within some sub-domains of an elastic or a piezoelectric medium can be considered as eigenfields which induce purely elastic or piezoelectric fields within the entire medium, Mura (1987), Shodja and Rashidinejad, (2014). The constitutive relations pertinent to a piezoelectric medium with arbitrary distribution of initial eigenstrain field, $\boldsymbol{\varepsilon}^*$ and eigenelectric field, $\boldsymbol{E}^*$ are given by

$$\sigma_{ij} = C_{ijkl}\left(\varepsilon_{kl} - \varepsilon_{kl}^*\right) - e_{kij}E_k, \quad i, j, k, l = 1,2,3, \tag{1}$$

$$D_j = \kappa_{kj}(E_k - E_k^*) + e_{jkl}\varepsilon_{kl}, \quad j, k, l = 1,2,3, \tag{2}$$

where σ, ε, D, and E are the stress, strain, electric displacement, and electric fields, respectively, and C, e, and κ are, respectively, the elastic moduli, piezoelectric, and dielectric tensors. In addition, the equilibrium equations and charge equation of electrostatics in the absence of external body forces and charges are

$$\sigma_{ij,j} = 0, \tag{3}$$

$$D_{j,j} = 0. \tag{4}$$

The strain and electric fields in (1) and (2) are written in terms of the derivatives of the elastic displacement field, u and electric potential field, Φ, respectively, as

$$\varepsilon_{kl} = \frac{1}{2}\left(u_{k,l} + u_{l,k}\right), \tag{5}$$

$$E_k = -\Phi_{,k}. \tag{6}$$

Therefore, by virtue of Eqs. (1)-(6), the governing partial differential equations pertinent to a piezoelectric medium including some QNSs can be expressed in terms of the elastic displacement and electric potential fields and initial eigenstrain and eigenelectric fields as:

$$C_{ijkl}u_{k,lj} + e_{kij}\Phi_{,kj} = C_{ijkl}\varepsilon^*_{kl,j}, \quad i, j, k, l = 1, 2, 3, \tag{7}$$

$$e_{jkl}u_{k,lj} - \kappa_{kj}\Phi_{,kj} = \kappa_{kj}E^*_{k,j}, \quad j, k, l = 1, 2, 3. \tag{8}$$

By utilization of the electro-mechanical eigenfield concept as described by Shodja and Rashidinejad (2014), periodically distributed QNSs may be modeled as periodic distribution of eigenfields expressed in terms of Fourier series with periods 2L1, 2L2, and 2L3 in the x1-, x2-, and x3-directions, respectively, as

$$\varepsilon^*_{kl}\left(\boldsymbol{x}\right) = \sum_{\xi}\bar{\varepsilon}^*_{ij}\left(\xi\right)\exp\left(i\xi.\boldsymbol{x}\right), \tag{9}$$

$$E^*_{k}\left(\boldsymbol{x}\right) = \sum_{\xi}\bar{E}^*_{k}\left(\xi\right)\exp\left(i\xi.\boldsymbol{x}\right), \tag{10}$$

where

$$\bar{\varepsilon}^*_{kl}\left(\xi\right) = \frac{1}{8L_1L_2L_3}\int_{\Omega}\varepsilon^*_{kl}\left(\boldsymbol{x}'\right)\exp\left(-i\xi.\boldsymbol{x}'\right)d\boldsymbol{x}', \tag{11}$$

$$\bar{E}^*_{k}\left(\xi\right) = \frac{1}{8L_1L_2L_3}\int_{\Omega}E^*_{k}\left(\boldsymbol{x}'\right)\exp\left(-i\xi.\boldsymbol{x}'\right)d\boldsymbol{x}', \tag{12}$$

$i=\sqrt{-1}$, ξ is the wave vector for given periods in different directions, and Ω is the volume of the QNS in a single period. Hence, due to the periodic nature of the problem, the elastic displacement and electric potential fields take on the series form

$$u_k(\boldsymbol{x})=\sum_{\xi}\bar{u}_k(\xi)\exp(i\boldsymbol{\xi}.\boldsymbol{x}), \tag{13}$$

$$\Phi(\boldsymbol{x})=\sum_{\xi}\bar{\Phi}(\xi)\exp(i\boldsymbol{\xi}.\boldsymbol{x}). \tag{14}$$

Substituting (9), (10), (13), and (14) into the governing partial differential equations (7) and (8) results in deriving the following governing equations in the Fourier space as

$$C_{ijkl}\xi_l\xi_j\bar{u}_k(\xi)+e_{kij}\xi_k\xi_j\bar{\Phi}(\xi)=-iC_{ijkl}\xi_j\bar{\varepsilon}^*_{kl}(\xi), \tag{15}$$

$$e_{jkl}\xi_l\xi_j\bar{u}_k(\xi)-\kappa_{kj}\xi_k\xi_j\bar{\Phi}(\xi)=-i\kappa_{kj}\xi_j\bar{E}^*_k(\xi), \tag{16}$$

for the Fourier coefficients of the elastic displacement and electric potential fields. Subsequently, the components of the coefficients matrix corresponding to the linear system of algebraic equations (15) and (16) are defined as:

$$K_{ik}(\xi)=K_{ki}(\xi)=C_{ijkl}\xi_l\xi_j, \tag{17}$$

$$K_{i4}(\xi)=K_{4i}(\xi)=e_{kij}\xi_k\xi_j, \tag{18}$$

$$K_{44}(\xi)=-\kappa_{kj}\xi_k\xi_j \tag{19}$$

Now by simultaneous solution of the equations (15) and (16), the elastic displacement and electric potential fields can be obtained in the series form as

$$u_i(\boldsymbol{x})=-i\sum_{\xi}[C_{jklm}\xi_k\bar{\varepsilon}^*_{lm}(\xi)N_{ij}(\xi)+\kappa_{kj}\xi_j\bar{E}^*_k(\xi)N_{i4}(\xi)]D^{-1}(\xi)\exp(i\boldsymbol{\xi}.\boldsymbol{x}), \tag{20}$$

$$\Phi(\boldsymbol{x})=-i\sum_{\xi}[C_{jklm}\xi_k\bar{\varepsilon}^*_{lm}(\xi)N_{4j}(\xi)+\kappa_{kj}\xi_j\bar{E}^*_k(\xi)N_{44}(\xi)]D^{-1}(\xi)\exp(i\boldsymbol{\xi}.\boldsymbol{x}), \tag{21}$$

in which Nij(ξ), i,j=1,2,3,4 and $D(\xi)$ are the cofactors and determinant of the 4×4 matrix $\boldsymbol{K}(\xi)$. Eqs. (20) and (21) provide the coupled electro-mechanical induced fields within a piezoelectric barrier in which the QNSs are periodically grown. After obtaining the mechanical displacement and electric potential fields via Eqs. (20) and (21), the strain and electric fields will be calculated from (5) and (6) and subsequently, Eqs. (1) and (2) can be utilized to obtain the stress and electric displacement fields. In the next section, by employment of the presented formulations, the induced electro-elastic fields due to periodically grown pyramidal QDs with different periodicities will be calculated and discussed.

3. Periodically grown pyramidal QDs: studying the effects of periodicity of the distribution

QDs with pyramidal geometries grown periodically via Stranski-Krastanov growth mode or molecular beam epitaxy (MBE) have been observed and studied by many investigators such as Bimberg et al. (1999) and Xu et al. (2007). Due to the lattice mismatch of the QDs and surrounding barrier, periodic distribution of QDs will induce electro-elastic fields within the QDs as well as the surrounding piezoelectric barrier. Since accurate determination of the electro-elastic fields in QNSs is a substantial issue for employment of these structures in optoelectronic and microelectronic devices, the present section is devoted to studying the induced electro-elastic fields in QNSs consisting of periodic distribution of pyramidal QDs with various periodicities. Short periodicities correspond to high-density QD structures while long periods refer to low-density ones. In order to study the effects of the density of QD structures, periodic distribution of square-based pyramidal QDs with base length of 20 nm and height of 5 nm is assumed (see Bimberg et al. (1999)). The QDs and the piezoelectric barrier are assumed, respectively, as indium nitride and aluminium nitride for which the material constants are given by Shodja and Rashidinejad (2014). The square-bases of pyramidal QDs are considered to be within or parallel to x1-x2 plane while their altitudes coincide with the axis of rotational symmetry and polarization of the piezoelectric barrier. The x1-x2 coordinates are located at the center of the square-base of one of the pyramids such that x1 and x2 axes are parallel or perpendicular to the edges of the QDs passing through the centers of other square-bases of pyramids in x1 and x2 QD arrays. Three different periods of 100 nm, 50 nm, and 30 nm in all the three directions are considered for periodic distribution of pyramidal QDs. It should be noted that the present formulation is capable of treating the problems in which periods in different directions are not equal. The initial misfit strain components distributed within the QDs are given by Jogai (2001) as

$$\varepsilon_{ij}^{*}\left(\boldsymbol{x}\right)=0.14\ \delta_{ij}. \tag{22}$$

Associated to the described distributions of pyramidal QDs, the Fourier coefficients of the initial misfit strains within QDs can be obtained as

$$\begin{aligned}
&\bar{\varepsilon}_{ij}^{*}\left(\xi\right)=\frac{0.14\delta_{ij}}{4L^{3}\ \xi_{1}\xi_{2}}\times\\
&\Big(\frac{2\mathrm{Sin}\left[10\left(\xi_{1}-\xi_{2}\right)\right]\left(\xi_{1}-\xi_{2}\right)+\mathrm{i}\mathrm{Cos}\left[10\left(\xi_{1}-\xi_{2}\right)\right]\xi_{3}}{4\left(\xi_{1}-\xi_{2}\right)^{2}-\xi_{3}^{2}}\\
&-\frac{2\mathrm{Sin}\left[10\left(\xi_{1}+\xi_{2}\right)\right]\left(\xi_{1}+\xi_{2}\right)+\mathrm{i}\mathrm{Cos}\left[10\left(\xi_{1}+\xi_{2}\right)\right]\xi_{3}}{4\left(\xi_{1}+\xi_{2}\right)^{2}-\xi_{3}^{2}}\\
&-\frac{16\mathrm{i}e^{-5\mathrm{i}\xi_{3}}\xi_{1}\xi_{2}\xi_{3}}{16\left(\xi_{1}^{2}-\xi_{2}^{2}\right)^{2}-8\left(\xi_{1}^{2}+\xi_{2}^{2}\right)\xi_{3}^{2}+\xi_{3}^{4}}\Big)
\end{aligned} \tag{23}$$

in which 2L indicates the period corresponding to each of the considered three different periodicities. By substituting Eq. (23) into Eqs. (20) and (21) and then using Eqs. (1), (2), (5) and (6), the coupled electro-elastic fields due to periodic distribution of pyramidal QDs with different periodicities can be determined. For demonstration, the variations of the strain component ε11 along x1-axis is shown in Fig. 1 for three different periods of 2L=100 nm, 2L=50 nm, and 2L=30 nm. It should be noticed that due to the symmetry in geometry and electro-mechanical properties of the problem, variations of the strain component ε22 along x2 would be the same as those of ε11 along x1. These variations interestingly reflect that periodic distribution of QDs may highly affect the electro-elastic fields within the QDs as well as the surrounding barrier. Effects of the periodically distributed QDs on the induced electro-elastic fields will be more significant for shorter periodicities; this occurs as a result of interactions between the quantum structures. Moreover, it can be observed that as the period of the distribution becomes shorter, the strain component ε11 within the QD regions will decrease while the absolute value of the strain component ε11 increases at the point within the surrounding barrier. It is clearly seen that in contrast to the periods of 100 nm and 50 nm, for the period of 2L=30 nm the strain component within the surrounding barrier never experiences small values. Interestingly, increasing the density of the quantum structures by decreasing the periodicity of their distribution leads to more considerable influence on the electro-elastic fields within the surrounding barrier in comparison with the quantum structures. A maximum change of 53 percent in the strain component ε11 occurs within the pyramidal quantum dots near the boundaries when the period of the distribution decreases from 100 nm to 30 nm.

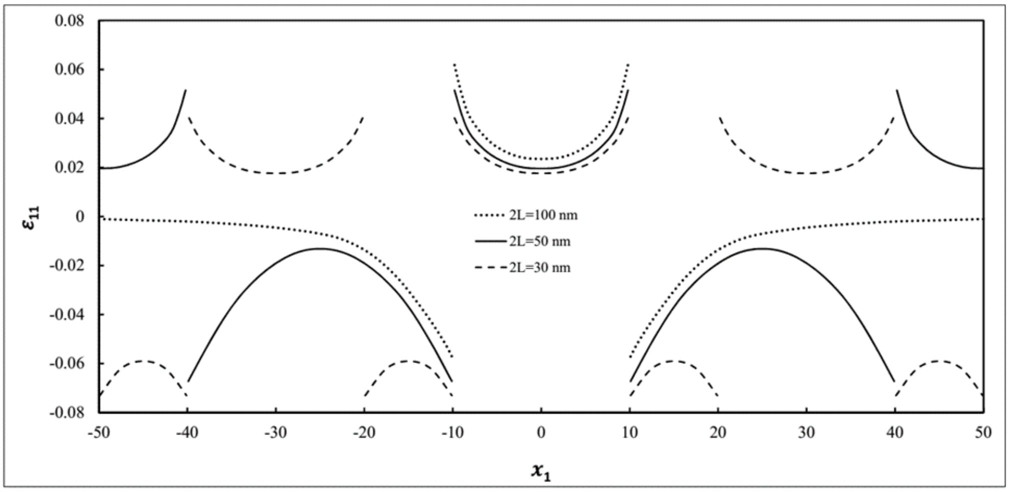

Fig. 1. Variations of the total strain component ε_{11} along x_1-axis for three different periods of 100 nm, 50 nm, and 30 nm.

4. Conclusions

An analytical formulation for accurate determination of the electro-elastic fields induced in QNSs is given and effects of periodicity of the pyramidal QDs on the induced fields are studied and discussed. The interactions of QNSs as well as the electro-mechanical couplings of the piezoelectric barrier are exhibited. The strain field of periodically distributed pyramidal QDs and the effects of their periodicity are studied which is of great value in design of QNSs. A maximum relative difference of approximately 53 percent in the stain component ε_{11} near the boundaries of periodically grown pyramidal QDs with periods of 30 nm and 100 nm is captured. It has been shown that for pyramidal QDs with base length of 20 nm, when the period of distribution is 50-100 nm the strain field component within the surrounding barrier experiences small values while the absolute value of the strain field component within the surrounding barrier does not decrease considerably for the period of 30 nm. As demonstrated, periodicity of distribution of the periodically grown pyramidal QDs affects the induced electro-elastic fields significantly and therefore, knowledge of the density of periodically grown QNSs would be of great importance in design and application of such structures.

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