Elastic analysis of an inhomogeneous quantum dot in multilayered semiconductors using a boundary element method

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In this work, we examine the elastostatic field due to a buried quantum dot (QD) in multilayered semiconductors using a boundary element method. Since the integral kernels employ a special Green's function that satisfies the interfacial continuity and boundary conditions for a multilayered matrix, coupled with the conventional Kelvin-type Green's function for the QD, the present method only requires discretization along the interface between the matrix and QD to solve the problem. With this method, the QD can be modeled in general as an inhomogeneity relative to the matrix. We have examined a practical semiconductor multilayer system of an InAs wetting/GaAs spacer with a buried cuboidal QD of either wetting or a spacer medium. The QD is correspondingly modeled by either the inhomogeneity or inclusion approach. Two crystallographic orientations of the spacer medium, GaAs(001) and GaAs(111), are considered. The analytical results have shown that these two approaches generally result in considerable differences in the prediction of the QD-induced elastic field. Also, different crystallographic orientation of a spacer medium can cause a characteristic change in the QD-induced field.
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I. INTRODUCTION

Self-assembled semiconductor heterostructures of quantum islands have attracted tremendous attention in recent years. The processing of the heterostructures is based on Stranski–Krastanow spontaneous growth of small surface islands from a wetting layer that is restrained to a lattice-mismatched substrate. The islands include quasizero-dimensional dots [or quantum dots (QDs)] and quasione-dimensional wires on the nanoscale. They are later covered by a thin layer of different medium, nominally, a spacer layer. Experimental studies have shown that the nanostructures with embedded QDs possess certain special electronic and optical features, rendering possible fascinating novel devices, such as low-threshold lasers, resonant tunneling devices, and huge-capacity memory media.[1] Since these features are in part related to the strain fields induced by the QDs, it would be essential to understand the latter before the design of devices. In the advancement of technology that utilizes the special electronic and optical features, multilayering of the QD nanostructures is often desirable.[2–6] To accurately and efficiently predict the strain field in such heterogeneous anisotropic media with multiple interacting nanoparticles still poses a great challenge to the research societies of physics and engineering.

The (buried) QDs have been approached by point source,[2,7] finite-sized inclusion,[8–13] and finite-sized inhomogeneity[14–17] of eigenstrains embedded in a matrix. In the first point-source approach, the effect of the finite geometry of QDs is not taken into account, which is appropriate only if the QD size is sufficiently small relative to all other length scales including the spacing of neighboring QDs and the thickness of spacer layer that covers the QDs. In the second inclusion approach, the geometry of QDs is taken into account, and the materials property is assumed to be identical to that of the spacer medium. By assuming this in these approaches, an analytical Green's function method may be derived to evaluate the induced strain fields upon the availability of the point-force Greeen's functions for the specific configuration. The numerical finite element (FE) and finite difference (FD) methods may also be used to solve the point-source and finite-size inclusion problems. The last inhomogeneity approach takes into account the effect of dissimilar materials properties between QDs and the spacer as well as the effect of finite geometry of QDs. The QDs usually are assumed to contain a medium identical to that of the wetting layer. In this case, the strain field of QDs has been solved numerically by using the FE[15,17] and FD[14,16] methods. All of these approaches discussed above are based on the local continuum assumption of matter, which has commonly been accepted in analyses of long-range fields of QDs.[1,18]

The short-range fields of QDs can be examined by using an atomic-level approach.[19–21] Daruka *et al.*[19] applied classical molecular dynamics (MD) simulation to examine the surface stress distribution in a Ge/Si QD superlattice. They found good agreement of their MD simulation results with analytical expressions based on the continuum force-dipole model. However, Makeev and Madhukar[20] reported a characteristic discrepancy between predictions of the dependence of hydrostatic stress on spacer thickness and island dimensions using those two approaches. Generally speaking, an atomic-level approach would be required from the perspective of predicting the elastic constants, mass transport coefficients, shapes, compositions, etc., of QDs and understand-

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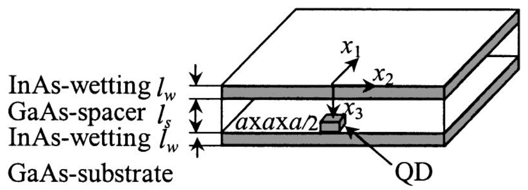

FIG. 1. Multilayered semiconductor system of InAs wetting/GaAs spacer/InAs wetting/GaAs substrate with a buried cuboidal QD of dimensions $a \times a \times a/2$.

ing the underlying physics in the process of QD formation. However, the computational expense normally is extremely high, thus prohibiting a simulation of QD nanostructures of large size or over the long term. A strategy for combining the continuum and atomic-level approaches, i.e., a quasicontinuum approach,[22] may in practice be feasible.

In this article, we apply a continuum-based boundary element (BE) method to examine the elastic strain fields of a generally inhomogeneous QD in multilayered semiconductors. Compared to the domain-based FE and FD methods, the BE method has the following general advantages. First, the problem of dimensionality is reduced by one. Second, the interior domain is not discretized because there the governing equation is satisfied exactly. Finally, if any stress concentration or singularity exists, it can be more accurately and conveniently modeled. Note that the last advantage is significant in the modeling of QDs where cuboidal and pyramidal shapes are often assumed. At the edges and corners of these geometries, stress singularity appears. Compared to conventional ones, the unique characteristic of the present BE method is the utilization of a special Green's function that satisfies the interfacial continuity and boundary conditions for the multilayered matrix,[23,24] coupled with the conventional Kelvin-type Green's function for the QD. This feature allows us to design the BE method without involving the interfaces and surfaces of the matrix unless a different situation occurs. In the other words, the present BE analysis of a generally inhomogeneous QD in multilayered semiconductors needs to numerically discretize only the interface between the matrix and QD.

In Sec. II, the formulation of a cuboidal QD in a multilayered matrix is described. In Sec. III, the BE method is first validated by comparing the numerical results of an inclusion QD to the analytical result by the Green's function method.[13] Then, it is applied to examine the effect of inhomogeneity of a buried QD relative to the embedding spacer medium on induced elastic field. We have investigated a semiconductor system of InAs wetting/GaAs spacer with two different crystallographic orientations of the spacer medium. It is shown that the effect of the inhomogeneity of a QD is significant in this semiconductor system. Also, different crystallographic orientation of the spacer medium can cause characteristic changes in the QD-induced elastic field. In Sec. IV, conclusions based on this study are drawn.

II. FORMULATION

Let us consider the problem of a cuboidal QD embedded in a multilayered half space of an InAs wetting/GaAs spacer/InAs wetting/GaAs substrate, shown in Fig. 1. The Cartesian coordinate system, (x_1, x_1, x_3), is chosen such that the x_3 axis is perpendicular to the matrix surface and that the origin (0, 0, 0) is on the top surface right above the center of the QD. The crystallographic directions [100], [010], and [001] of the InAs crystals are taken to be along the global coordinates x_1, x_2, and x_3, respectively. The crystallographic orientations of the GaAs crystals will be specified later. The QD is on the top surface of the interior InAs-wetting layer and covered by the GaAs-spacer layer. The sides of the cuboidal QD are taken to be along the global coordinates, x_1, x_2, and x_3, respectively. The interfaces between the different subdomains all are perfectly bonded. The matrix surface is free of traction. The eigenstrain in the QD is assumed to be uniform and hydrostatic, i.e., $\varepsilon_{ij}^0 = \varepsilon^0 \delta_{ij}$, and that in the matrix layers to be zero. Note that in reality, the wetting layers should also have uniform distribution of nonzero eigenstrain, similar to the QD. In this case, the field to be derived under the above condition of zero eigenstrain in the multilayered matrix is actually the part of the field induced by the QD. The total field can be obtained by applying the rule of superposition of the induced field to the homogeneous field that is derived as if there were no QD but with the matrix eigenstrain under the same boundary and interfacial conditions. The elastic constants for GaAs are $C_{11} = 118$, $C_{12} = 54$, and $C_{22} = 59$ and for InAs are $C_{11} = 83$, $C_{12} = 45$, and $C_{22} = 40$ (GPa) in their crystallographic base axes. The dimensions of the cuboidal QD are $a \times a \times a/2$. The thickness of both the wetting layers, l_w, is equal to $0.1a$ while the spacer thickness, l_s, will be varied in later simulations.

To solve the problem shown in Fig. 1, we apply the nonconventional multilayered BE method to the semiconductor multilayers discussed above, coupled with the conventional BE method using the Kelvin-type fundamental solution to the QD. The present BE method is developed based on the following boundary integral-equation formulation:

$$c u_i^{(M)}(\mathbf{X}) = \int_{\partial M} \Big[u_{ij}^{*(M)}(\mathbf{X},\mathbf{x}) p_j^{(M)}(\mathbf{x}) - p_{ij}^{*(M)}(\mathbf{X},\mathbf{x}) \times u_j^{(M)}(\mathbf{x}) \Big] dS(\mathbf{x}) \tag{1}$$

for the multilayered matrix, and

$$c u_i^{(D)}(\mathbf{X}) = \int_{\partial D} \Big\{ u_{ij}^{*(D)}(\mathbf{X},\mathbf{x}) \big[p_j^{(D)}(\mathbf{x}) - F_j^{(D)}(\mathbf{x}) \big] - p_{ij}^{*(D)}(\mathbf{X},\mathbf{x}) u_j^{(D)}(\mathbf{x}) \Big\} dS(\mathbf{x}) \tag{2}$$

for the buried QD, where $F_j^{(D)} = C_{jklm}^{(D)} \varepsilon_{lm}^0 n_k$, in which C_{ijlm} is the elastic stiffness tensor, and n_k is the unit outward normal at a boundary point. The coefficient c is equal to 1 if $\mathbf{X}$ is an interior point and to 0.5 if $\mathbf{X}$ is a boundary point (except for sharp corners). The fundamental solutions $u_{ij}^{*(M)}$ and $p_{ij}^{*(M)}$ are the special Green's functions for anisotropic multilayers.[23,24] Meanwhile, $u_{ij}^{*(D)}$ and $p_{ij}^{*(D)}$ are Green's functions for infinite space of an anisotropic medium.[25] The expressions for strain and stress can be obtained by taking derivatives of Eqs. (1) and (2) and applying Hooke's law. For details of the numerical issues of how to construct a discrete

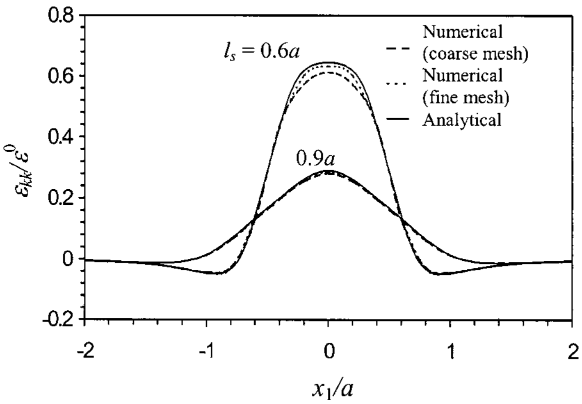

FIG. 2. Convergence check of the numerical BE solution of an inclusion QD compared tothe analytical solution by the Green's function method.

version of the above boundary integral-equation formulation and an algorithm to solve it, one can refer to the work of Brebbia *et al.*[26] We have adopted the iterative scheme of successive overrelaxation to solve the present BE problem.[27] In the following, we shall first verify our formulation by comparing the BE solution of an inclusion QD to the available analytical solution by the Green's function method using the same multilayered Green's functions.[13] After validation, the effect of inhomogeneity of a buried QD relative to the embedding spacer is examined. Two crystallographic orientations of the spacer medium, GaAs(001) and GaAs(111), will be considered, where the index indicates the crystallographic orientation in the x_3 direction.

III. ANALYSIS

In order to validate our formulation, we first take the QD as an inclusion, assuming that the QD consists of the same medium as the matrix it occupies, i.e., the spacer. In this case, the strain field can be solved analytically by using the Green's function method.[13] The spacer and QD are substituted by the GaAs(001). The QD-induced hydrostatic strain along a line $(x_1, 0, 0)$ on the surface obtained, respectively, by the analytical method and by the numerical BE method with two different meshes are compared in Fig. 2. The coarse mesh is $5\times5\times3$ divisions, respectively, along the three sides of the QD while the finer mesh is $10\times10\times5$ divisions. The constant interpolation function is used in each of the resulting rectangular elements. The spacer thickness is indicated in Fig. 2. It can be seen that the numerical solutions are close to the analytical solutions, even with the quite coarse mesh. When the mesh is refined, the numerical BE solution approaches the analytical solution, indicating the convergence of the numerical solution with mesh refinement. These features have demonstrated the validity of the present formulation. We want to remark that the computational time for the strain field using the analytical Green's function method is much shorter than that using the numerical BE method. In the numerical BE method, the solution is obtained in two steps: solving the fields along the interface between the QD and multilayered matrix, and then calculating the fields at desired locations in postprocessing. In the analytical Green's function method, the solution procedure comprises only the computation of an integral that corresponds to the second step in the former. Therefore, if the QD can be approached as an inclusion, the Green's function method is more desirable than the numerical BE method. On the other hand, should the QD be approached as inhomogeneity, the numerical BE method (or other numerical methods) needs to be adopted in a trade-off of computational efficiency. Below, we examine how necessary it is to model a buried QD as inhomogeneity against inclusion in the semiconductor system of InAs/GaAs.

We now consider the same multilayered semiconductor system as above. At this time, however, the QD is assumed to contain the same medium as the InAs-wetting layer (instead of the GaAs spacer) in the inhomogeneity approach. This approach of QDs is considered to be a more realistic approximation than the inclusion approach due to the fact that the QD is grown from the wetting layer via mass transport but covered by the foreign spacer medium. However, we note that even the assignment of the same medium of the parent wetting layer to the QD may not make an exact approach to the problem because the QD growth, as normally believed, is of the diffusional type of phase transition that involves a change in composition at a mass point. In other words, the QDs may have different compositions and hence difference materials properties than the wetting layer. The evaluation of the elastic property of QDs, either experimental or theoretical, remains a great challenge to researchers because of the small scales. Figure 3 shows the variation of hydrostatic strain ε_{kk} along $(x_1, 0, 0)$ on the top surface of the QD at three different values of spacer thickness compared to the result by the inclusion approach. Note that in this example, the GaAs(001) is used for the spacer and substrate while the InAs(001) is used for the wetting layers and QD. All other parameters are kept the same as in the previous simulation. It can be seen that the hydrostatic strain shows a maximum value at the origin (0, 0, 0) right above the center of the QD in the first two cases of spacer thickness equal to 0.6a [Fig. 3(a)] and 1.2a [Fig. 3(b)]. In the third case of spacer thickness, equal to 2.2a [Fig. 3(c)], the profile of hydrostatic strain has gone through a transition from convex to concave at the top region. Meanwhile, the amplitude of hydrostatic strain rapidly decreases with an increase in spacer thickness. Due to the symmetry of the materials and the QD shape, the field induced over the QD is symmetric relative to the x_2 axis as well as to the x_1 axis (not shown). Compared to the inclusion solution, it is seen that in the case of spacer thickness equal to 0.6a, which is small compared to the QD height of 0.5a, there appears not to be much difference between the two solutions. The relative difference is rather obvious at larger spacer thickness. Because the spacer medium is elastically stiffer than the wetting medium, the peak value of hydrostatic strain over the CD is larger by the inhomogeneity approach than by the inclusion approach.

Finally, we examine the elastic field of a buried QD in the multilayered semiconductor system with the spacer and substrate medium being substituted by the GaAs(111). Similar to in the previous analysis, the surface hydrostatic strain field over the cuboidal QD is obtained with the QD being approached as either inclusion or inhomogeneity. The results for three different values of spacer thickness are plotted in

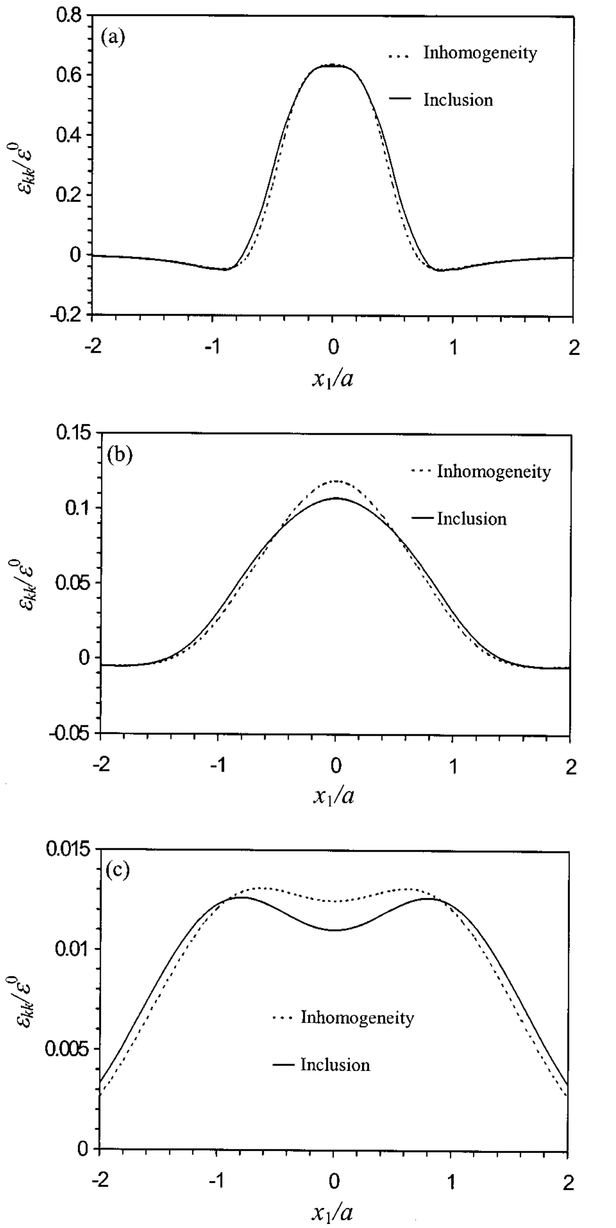

FIG. 3. Variation of normalized hydrostatic strain ($\varepsilon_{kk}/\varepsilon^0$) along ($x_1$, 0, 0) over the QD at various values of spacer thickness l_s: (a) 0.6*a*; (b) 1.2*a*; (c) 2.2*a*. The solutions by the approaches of inhomogeneity and inclusion are compared. The spacer is substituted by the GaAs(001).

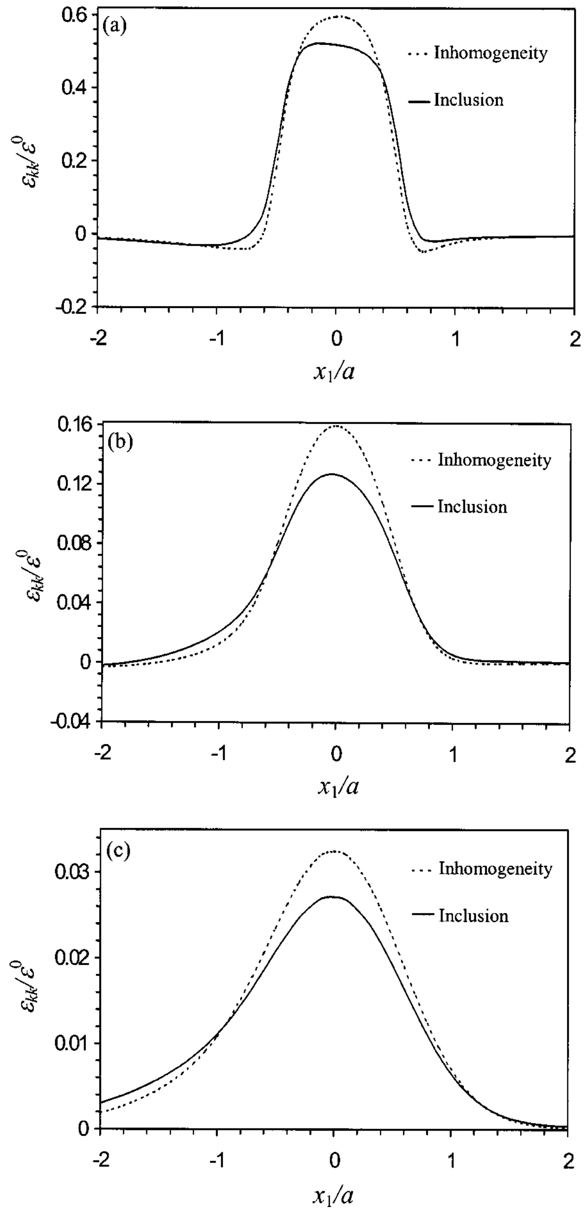

FIG. 4. Variation of normalized hydrostatic strain ($\varepsilon_{kk}/\varepsilon^0$) along ($x_1$, 0, 0) over the QD at various values of spacer thickness l_s: (a) 0.6*a*; (b) 1.2*a*; (c) 2.2*a*. The solutions by the approaches of inhomogeneity and inclusion are compared. The spacer is substituted by the GaAs(111).

Fig. 4. In comparison to the plots in Fig. 3 for spacer and substrate made of the GaAs(001), several distinct features can be observed. First, the hydrostatic strain profile over the QD is asymmetric relative to the x_2 axis, but symmetric relative to the x_1 axis which is not shown. Second, the effect of QD inhomogeneity on the elastic field is pronounced for all three values of spacer thickness. Finally, the transition from convexity to concavity of the hydrostatic strain field above the QD with respect to spacer thickness is not observed in the case of the GaAs(111) as the spacer and substrate.

IV. CONLCUION

We have examined the elastic field of a buried QD in multilayered semiconductors by applying a BE method. Since the integral kernels employ the special Green's function that satisfies the interfacial and boundary conditions of the multilayered matrix, the present BE method only requires discretization along the interface between the matrix and QD to solve the problem. With this method, the QD can be modeled in general as inhomogeneous relative to the matrix. As an example, we have examined the practical semiconductor multilayer system of InAs wetting/GaAs spacer with a cuboidal QD. The QD was modeled as either inclusion or inhomogeneity in two crystallographic orientations of spacer, GaAs(001) and GaAs(111). By comparing the numerical inclusion solution to the analytical solution by the Green's function method, the present formulation has been validated. Also, by comparing the results by the two approaches of inclusion and inhomogeneity, it has been shown that these approaches generally result in considerable differences in the prediction of the QD-induced elastic field. Also, different crystallographic orientation of a spacer medium can cause a characteristic change in the field.

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