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Green's tensors for anisotropic elasticity: Application to quantum dots

D. A. Faux and G. S. Pearson
Department of Physics, University of Surrey, Guildford GU2 7XH, United Kingdom
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Real-space Green's tensors for the calculation of the strain in systems containing buried quantum dots of arbitrary shape and composition, including the cubic anisotropy of elastic constants, are presented, to the best of our knowledge, for the first time. The Green's tensors are obtained as a series with very good accuracy obtained using the first two terms. The Green's function for the hydrostatic strain is of a simple form and it is shown that the cubic anisotropy leads to a nonzero hydrostatic strain outside a dot. The axial strain is shown to depend on the orientation of the dot in the crystal.

There is considerable experimental and theoretical interest in semiconductor quantum dot (QD) structures because devices offer the prospect of improved electronic and optical properties arising from the zero-dimensional quantum confinement of carriers.[1] Knowledge of the *strain* distribution in and around individual QD's is essential input to calculations of the electronic and optical properties of devices,[2–6] transmission electron microscopy (TEM) image simulation,[7,8] and crucial for the understanding of the mechanics of growth.[9–11]

The calculation of the strain distribution due to a buried inclusion with uniform misfit is usually tackled using finite-element (FE) techniques.[2,3,7,8] However, these are computationally intensive, making it difficult to adjust parameters to obtain a best fit with experiment, the treatment of the boundary conditions requires care and QD arrays or QD's with compositional variation pose difficulties. Methods based on Green's functions, on the other hand, are generally quick, portable, large systems involving many QD's or dots with graded composition pose no difficulty and analytic expressions are sometimes tractable to provide deeper insight into the physics, revealing trends, and simple relations.[4–6,12–15] For example, full analytical expressions for the strain distribution have been derived for ellipsoidal, cuboidal, and truncated-pyramidal dots.[5,13]

The chief restriction of the Green's function approach is that isotropy of elastic constants is assumed. For some problems an isotropic solution may be justified because there are much greater uncertainties (such as dot size and shape) which dominate the accuracy of the calculation, or anisotropy is not significant for the phenomena under investigation.[7] Yet most semiconductors *are* cubic crystals with an anisotropy coefficient, defined in terms of the elastic constants by $(C_{11}-C_{12})/2C_{44}$, typically equal to 0.5 compared to the isotropic value of 1, suggesting that the simple isotropic approach may miss some key features of the strain field. For example, Holý *et al.* and Pinczolits *et al.* have demonstrated that the *lateral* ordering of QD's can be explained *only* if the full cubic anisotropy of the crystal is taken into account.[9,10] The most accessible strain analysis which includes the cubic anisotropy of elastic constants is by Andreev *et al.* who use a Fourier series method to obtain the lattice relaxation associated with a sinusoidal variation of lattice constant.[16] The Fourier series yields the strain distribution for an infinite array of evenly-spaced QD's which is semianalytic for most common QD shapes.[17] Even so, calculations are lengthy, accuracy depends on the number of Fourier terms, performing the calculation for a single QD or a QD with variable composition is troublesome, and the technique lacks the simplicity of applicability of the Green's function approach.

In this paper we present explicit real-space Green's tensors which enable the strain distribution in and around QD's to be calculated rapidly and accurately, including the cubic anisotropy of the elastic constants. Our expressions are derived from the work of Mura and Kinoshita[18] who described from first-principles how the Green's tensor for anisotropic elasticity can be determined in series form based on the work of Lifshits and Rosentsverg.[19]

In the summary which follows it is assumed, first, that the elastic properties are linear, second, the same elastic constant pertain to the QD and the surroundings (the use of the elastic constants of the barrier material for both barrier and QD has been justified elsewhere)[16,13] and, third, the QD is embedded in an infinite matrix. We obtain an expansion for the strain Green's tensor, $\boldsymbol{G}^{\epsilon\odot}$, of the form

$$\boldsymbol{G}^{\epsilon\odot}=\boldsymbol{G}_0^{\epsilon\odot}+\Delta\boldsymbol{G}_1^{\epsilon\odot}+\Delta^2\boldsymbol{G}_2^{\epsilon\odot}\cdots, \tag{1}$$

where the first term is the isotropic Green's tensor, $\boldsymbol{G}_0^{\epsilon\odot}$, and subsequent terms provide successive orders of correction converging to the full anisotropic result. The expansion coefficient $\Delta=\mu'/(\lambda+2\mu)$ where $\mu=C_{44}$, $\lambda=C_{12}$ are the usual Lamé constants and $\mu'=C_{11}-C_{12}-2C_{44}$. $\Delta\sim-\frac{1}{3}$ for typical semiconductor materials. Cubic crystals are isotropic when $\mu'=0$. The superscripts ''ϵ'' and ''$\odot$'' indicate that this Green's tensor yields the strain and is specific to QD's, respectively. All quantities in boldface are tensors.

The strain tensor is obtained by integrating the Green's tensor over the volume of the dot, thus

$$\boldsymbol{\epsilon}^{\odot}(x_1,x_2,x_3)=\int_V \boldsymbol{G}^{\epsilon\odot}(x_1',x_2',x_3')\,dV(x_1^{\odot},x_2^{\odot},x_3^{\odot}), \tag{2}$$

where $x_i'=x_i-x_i^{\odot}$ are Cartesian coordinates. Here the coordinate superscript ''$\odot$'' refers to points within the volume of the QD and V therefore represents the volume of the dot. The strain tensor can therefore be obtained for *any* QD shape.

We have found that the n^{th} term of the series, $\boldsymbol{G}_n^{\epsilon\odot}$, in Eq. (1) may be written

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$$\boldsymbol{G}_n^{\epsilon^\odot}=\frac{\boldsymbol{\epsilon}_0}{n!4^{n+1}\pi\mu^n(2\mu+\lambda)|\boldsymbol{x}|^{4n+5}}\begin{pmatrix} G_{n\parallel}^{\epsilon^\odot}(x_1,x_2,x_3) & G_{n\perp}^{\epsilon^\odot}(x_1,x_2,x_3) & G_{n\perp}^{\epsilon^\odot}(x_1,x_3,x_2) \\ \cdots & G_{n\parallel}^{\epsilon^\odot}(x_2,x_3,x_1) & G_{n\perp}^{\epsilon^\odot}(x_2,x_3,x_1) \\ \cdots & \cdots & G_{n\parallel}^{\epsilon^\odot}(x_3,x_1,x_2) \end{pmatrix}, \tag{3}$$

where the symbols $\parallel$ and $\perp$ indicate plane and shear strain components and the tensor elements are polynomial functions of coordinates of order $4n+2$. For example,

$$G_{0\parallel}^{\epsilon^\odot}(x_1,x_2,x_3)=-(2\mu+3\lambda)(|\boldsymbol{x}|^2-3x_1^2), \tag{4}$$

$$G_{0\perp}^{\epsilon^\odot}(x_1,x_2,x_3)=3(2\mu+3\lambda)x_1x_2, \tag{5}$$

where $|\boldsymbol{x}|^2=x_1^2+x_2^2+x_3^2$. Equations (4) and (5) combined with Eq. (3) with $n=0$ yield the well-known Green's functions for the plane and shear strain components, respectively, for isotropic crystals.

The higher-order terms are new results. The Green's functions for $n=1$ may be written,

$$G_{1\parallel}^{\epsilon^\odot}(x_1,x_2,x_3)=\sum_{i=0}^{3}\sum_{j=0}^{3-i}K_{ij}^{\epsilon^\odot}x_1^{2i}x_2^{2j}x_3^{6-2i-2j}, \tag{6}$$

$$G_{1\perp}^{\epsilon^\odot}(x_1,x_2,x_3)=x_1x_2\sum_{k=0}^{2}\sum_{i=0}^{2-k}L_{ki}^{\epsilon^\odot}x_3^{2k}x_1^{2i}x_2^{4-2i-2k}. \tag{7}$$

The constants $K^{\epsilon^\odot}$ and $L^{\epsilon^\odot}$ are presented in Table I. The functions comprising the $n=2$ Green's tensor are polynomials of order 10,

$$G_{2\parallel}^{\epsilon^\odot}(x_1,x_2,x_3)=\sum_{i=0}^{5}\sum_{j=0}^{5-i}M_{ij}^{\epsilon^\odot}x_1^{2i}x_2^{2j}x_3^{10-2i-2j}, \tag{8}$$

$$G_{2\perp}^{\epsilon^\odot}(x_1,x_2,x_3)=x_1x_2\sum_{k=0}^{4}\sum_{i=0}^{4-k}N_{ki}^{\epsilon^\odot}x_3^{2k}x_1^{2i}x_2^{8-2i-2k}, \tag{9}$$

where the constants $M^{\epsilon^\odot}$ and $N^{\epsilon^\odot}$ are listed in Table II. The first-order or second-order correction to a plane strain component can be calculated by substituting Eq. (6) or both Eqs. (6) and (8) into Eqs. (1)–(3) and integrating over the volume of the dot. The principle of superposition allows the strain in systems containing large numbers of QD's to be determined and composition variation within the QD is also easily catered for by making $\boldsymbol{\epsilon}_0$ a function of position and including it inside the integral. The numerical integration may be completed in minutes on a standard workstation, making these calculations several orders of magnitude faster than any alternative numerical technique. The ease and speed of the calculation opens up the possibility of using QD parameters such as size, shape, and composition profile as fit parameters in order to compare with experiment, for example, with TEM images.

It is important to establish how many terms of the series expansion given in Eq. (1) are necessary to provide an accurate determination of the strain including the cubic anisotropy of elastic constants. We therefore calculate the strain due to a spherical QD. Here, the difference between the iso-

TABLE I. The coefficients $K_{ij}^{\epsilon^\odot}$ (upper table) and $L_{ki}^{\epsilon^\odot}$ (lower table) are of the form $f(A\mu^2+B\mu\lambda+C\lambda^2)$ where μ and λ are the Lamé constants.

i	j	f	A	B	C
3	0	2	14	19	9
2	0,1	−9	14	35	17
1	0,2	9	6	19	15
	1	−36	2	3	0
0	0,3	−1	2	1	9
	1,2	6	4	12	3

k	i	f	A	B	C
2	0	3	22	51	39
1	0,1	−3	26	83	42
0	0,2	3	22	41	24
	1	−3	26	93	57

TABLE II. The coefficients $M_{ij}^{\epsilon^\odot}$ (upper table) and $N_{ki}^{\epsilon^\odot}$ (lower table) are of the form $f(A\mu^3+B\mu^2\lambda+C\mu\lambda^2+D\lambda^3)$ where μ and λ are the Lamé constants.

i	j	f	A	B	C	D
5	0	−2	−6	35	44	3
4	0,1	−1	1350	2477	2060	741
3	0,2	2	1860	7336	7405	2373
	1	4	1350	5611	4975	1158
2	0,3	−1	1690	7307	11080	4371
	1,2	3	1170	3223	340	−621
1	0,4	2	80	−74	−25	273
	1,3	−2	1270	5291	5755	1158
	2	6	150	197	380	621
0	0,5	1	2	−17	92	3
	1,4	5	14	−11	122	39
	2,3	−5	86	457	230	75

k	i	f	A	B	C	D
4	0	3	38	37	8	117
3	0,1	−6	374	1221	1524	531
2	0,2	3	818	3687	4248	1677
	1	8	176	1094	666	−81
1	0,3	−6	294	871	929	276
	1,2	2	784	5566	5499	981
0	0,4	3	118	177	78	57
	1,3	−2	1042	3103	3312	1233
	2	1	2054	10781	14004	5121

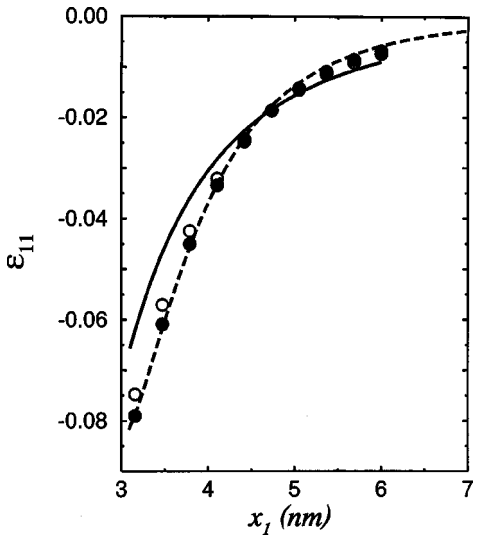

FIG. 1. The strain component, ϵ_{11}, is plotted as a function of x_1 for a spherical InAs QD of radius 3 nm contained in a GaAs matrix. Results for the region outside the dot, $x_1 > 3$ nm, are presented. The solid curve is the isotropic result. The dashed curve is the published result for an array of spherical QD's including the cubic anisotropy of elastic constants. The Green's function results include the first-order correction (○) and the second-order correction (●).

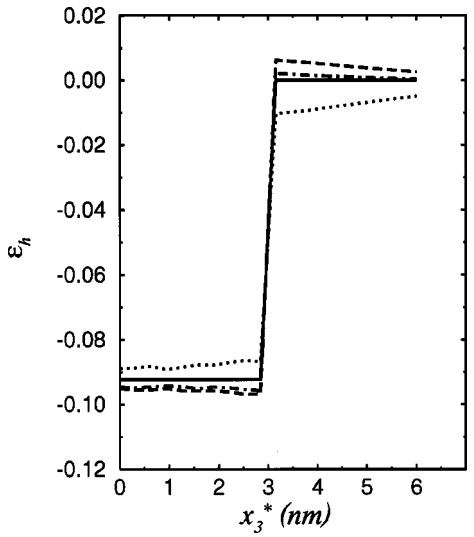

FIG. 3. The hydrostatic strain component, ϵ_h, plotted along the growth axis is presented for the cuboidal QD illustrated in Fig. 2 with $a=3$ nm. The solid line is the isotropic result. The remaining curves correspond to the growth direction along [001] (· · · · · · · ·), [110] (– · – – · – · –), and [111] (– – – – –).

tropic and anisotropic results is significant and the strain distribution is not complicated by geometrical effects. The elastic constants used for all materials are $C_{11}=118.8$ GPa, $\lambda=53.8$ GPa, and $\mu=59.4$ GPa corresponding to the values for GaAs.[20] The misfit strain, ϵ_0, is -0.067%. Figure 1 shows the strain component ϵ_{11} plotted as a function of x_1 including the first-order correction $G_0^{\epsilon\odot}+\Delta G_1^{\epsilon\odot}$ and the second-order correction $G_0^{\epsilon\odot}+\Delta G_1^{\epsilon\odot}+\Delta^2 G_2^{\epsilon\odot}$. We present results only for the region outside the QD because ϵ_{11} is constant and very close to the isotropic result *inside* the QD in all cases.[24] The results are compared to the calculations of Andreev *et al.* for an array of spherical dots with center-to-center separations of 18 nm using $200\times200\times200$ fourier terms. Figure 1 shows that the first-order correction provides a very good approximation to the strain. Addition of the second-order term provides an almost exact correspondence with the results of Andreev *et al.* We conclude that *only the zeroth- and first-order terms* of the strain Green's tensor expansion are required for good accuracy.

We now calculate the hydrostatic and axial strains for a cuboidal QD with growth direction along the x_3^* axis as illustrated in Fig. 2. Dimensions $a=3$ nm and $b=9$ nm are chosen because the 3:1 ratio is consistent with a range of QD's including the truncated pyramid characteristic of InAs/GaAs systems (for example, Fry *et al.*),[21] the lens or cylinder, and so these results illustrate the general trends to be found in a range of QD systems. Elastic constants for GaAs are again used for all materials and the misfit strain is taken to be -0.067%. We focus on three cases with the growth direction along [001], [110], and [111]. With the x_3^* axis aligned along [110], the x_1^* and x_2^* axes are taken to be along $[\bar{1}10]$ and [001], respectively, and when the x_3^* axis points along [111] the x_1^* and x_2^* axes are in the $[1\bar{1}0]$ and $[11\bar{2}]$ directions, respectively.

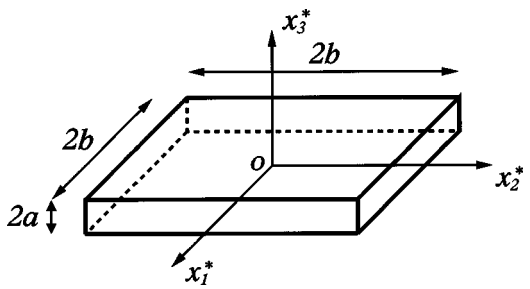

FIG. 2. The geometric parameters which define a cuboidal QD are illustrated. The growth direction is along x_3^*.

The hydrostatic strain is defined as $\epsilon_h=\epsilon_{1*}+\epsilon_{2*}+\epsilon_{3*}$, where the asterisk indicates the coordinate system illustrated in Fig. 2, and shifts the conduction band and average valence-band-edge energies.[22,23] We find that the Green's function for the first-order correction to ϵ_h for cubic crystals is of a particularly simple form

$$G_1^{\epsilon_h\odot}=\frac{3(2\mu+3\lambda)\epsilon_0}{4\pi(2\mu+\lambda)|\mathbf{x}|^7}\{x_1^4+x_2^4+x_3^4 - 3(x_1^2x_2^2+x_2^2x_3^2+x_3^2x_1^2)\}. \quad (10)$$

Figure 3 presents ϵ_h as a function of distance along the x_3^* axis through the center of the dot along [001], [110], and [111]. Inside the QD, ϵ_h is only a weak function of position and a weak function of growth direction and ranges from about -0.087 [001] to -0.097 [111] with the isotropic value equal to -0.092. Outside the QD, ϵ_h is zero in the isotropic approximation. Figure 3 demonstrates clearly that the cubic anisotropy of the elastic constants leads to nonzero hydrostatic strain outside the QD. ϵ_h is positive with a maximum value of 0.0062 for a QD grown on a (111) surface and larger and negative with a largest value of -0.01 for growth along the [001] axis. The hydrostatic strain will shift the conduction band and average valance-band energies and is

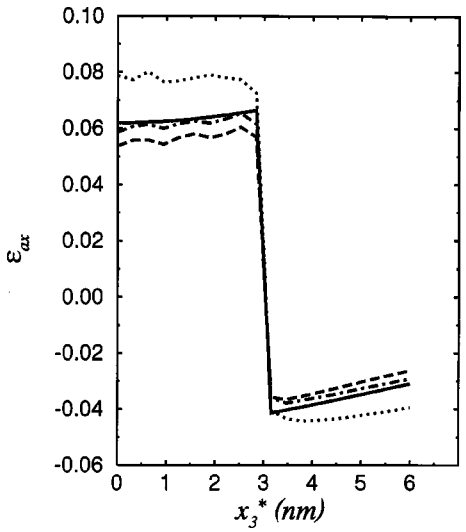

FIG. 4. The axial strain component, ϵ_{ax}, plotted along the growth axis is presented for the cuboidal QD illustrated in Fig. 2 with $a=3$ nm. The solid line is the isotropic result. The remaining curves correspond to the growth direction along [001] (· · · · · · · ·), [110] (– · – · – · –), and [111] (– – – – –).

significant over distances of the order of the dimension of the dot (about 6 nm outside the QD in this case).

Positive axial strain raises the energy of the heavy holes with respect to the light holes and vice versa. Figure 4 presents the axial strain, defined as $\epsilon_{\mathrm{ax}}=\epsilon_{3*}-\frac{1}{2}(\epsilon_{1*}+\epsilon_{2*})$, plotted as a function of distance along the growth axis. Inside the QD, ϵ_{ax} is typically 0.02 larger for a dot with a [001] growth direction compared to one grown along [111]. The orientation dependence of the axial strain increases with an increasing ratio of characteristic dimensions. For example, a cuboid with a 5:1 ratio of side dimensions possesses an axial strain of 0.096 and 0.071 for the [001] and [111] growth directions, respectively. These values are 0.128 and 0.098 in the quantum-well limit.[22] For both the hydrostatic and axial strain components, it is found that results are very similar to the isotropic solutions for a growth axis along the [110] direction.

In conclusion, the Green's tensors, in the form of a series, enabling the calculation of strain distributions in buried QD systems including the cubic anisotropy of the elastic constants are presented, to the best of our knowledge, for the first time. It is demonstrated that very good accuracy is achieved by including just the first-order correction enabling simple, fast, calculations of the strain distribution. QD's with composition variation are trivial extensions of the method. The Green's function for the first-order correction to the hydrostatic strain is shown to be of a particularly simple form and it is shown that the presence of cubic anisotropy introduces nonzero hydrostatic strain outside the QD which is positive for a QD grown on a (111) surface and negative for growth on a (001) surface. The axial strain is shown to be significantly dependent on the orientation of the dot.

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