Elastic and piezoelectric fields around a buried quantum dot: A simple picture

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Abstract

The elastic field around a buried, strained quantum dot is solved with a scalar potential that obeys Poisson’s equation. Standard methods from electrostatics can therefore be used. The lattice mismatch and displacement are analogous to the charge density and electric field. The dilation is proportional to the local lattice mismatch and therefore vanishes outside a dot. Expressions are also given for the piezoelectric potential. The results agree remarkably well with previous numerical calculations for a pyramidal dot. Thermoelasticity provides another analogy with many useful solutions available. These results are for an isotropic medium but cubic symmetry is considered briefly.

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I. INTRODUCTION

The inhomogeneous nature of semiconducting devices leads inevitably to stress within them, which couples to carriers through the band structure and piezoelectric effect. Homogeneously strained layers are used to improve the performance of devices such as lasers or pseudomorphic transistors. Inhomogeneous strain may arise from a patterned layer on the surface such as passivation, a metal gate or interconnect. This has been exploited to trap excitons below the surface. Lateral surface superlattices, devices with a periodic metal gate, are particularly sensitive to the built-in potential from stress and the angular dependence confirms that the piezoelectric effect is the dominant coupling for electrons.

The growth of self-assembled quantum dots in the Stranski–Krastnow mode provides a spectacular example where stress has been exploited. Take dots of InAs on a substrate of GaAs as an example. Their natural lattice constants differ by 7.2%, which causes a large stress to develop as a film of InAs forms on GaAs. This is partly relieved by the aggregation of InAs into dots of a roughly pyramidal shape. A large stress remains, however, so it is essential to consider the influence of stress on the properties of the dot and its surroundings.

Several methods can be used to calculate the stress. The elastic properties are usually assumed to be isotropic and homogeneous in analytic work but the results provide considerable insight despite these simplifications. Downes et al. used Eshelby’s theory of inclusions to express the stress in quantum wires and dots as an integral over their surface. Attractive results were found for rectangular wires and cuboidal dots. The next step is to include the cubic symmetry of the elastic behavior and the variation of elastic constants inside and outside the dot. Numerical solution is generally required but finite-element methods are well developed. This approach was used in the thorough analysis of a pyramidal dot by Grundmann et al. Finally, an atomistic approach should be taken at the smallest scale. The symmetry is further reduced; for example the [110] and [110] directions are not equivalent in the zinc-blende semiconductors. The large strains may also exceed linear elastic behavior and require a detailed model of the inter-atomic force.

This work extends the analytical approach in three dimensions for homogeneous, isotropic material. It is shown that the elastic field may be derived from a scalar potential that obeys a Poisson equation with the lattice mismatch as charge density. The displacement is analogous to the electric field and this provides a simple way to visualize the distortion around a dot. The dilation is a local function of the lattice mismatch and is therefore constant within a dot of constant composition, and vanishes outside. Another valuable analogy is with thermoelasticity, the distortion generated by a nonuniform temperature. Many useful solutions are available, including the effect of a plane surface. The elastic properties of GaAs are significantly anisotropic so the effects of cubic symmetry are considered briefly, mainly to find an appropriate value for Poisson’s ratio in the equations for isotropic behavior. The piezoelectric potential is then deduced from the elastic field. It is generally weak within a dot but provides the only coupling to electrons outside. A surface integral is derived, analogous to that for the stress. The strain and piezoelectric potential are calculated for a pyramid and agree remarkably well with numerical work.

The main assumptions in these calculations are as follows. The example of an InAs dot in GaAs will be used for definiteness. This has only a single conduction band unlike some other strained systems, notably Si–Ge.

1. The elastic behavior is linear and isotropic, with the same elastic constants everywhere.
2. The dot is embedded in an infinite medium with no surfaces to perturb the elastic field.
3. The structure is conformal, meaning that it can be obtained by starting from a perfect crystal of GaAs and locally transmuting the Ga atoms into In.

4. All distortions are measured with respect to the lattice constant of unstrained GaAs. This introduces some errors because the strains in InAs should be measured with respect to the lattice constant of InAs, not that of GaAs. The difference is of second order and the error is likely to be less than those due to other assumptions, but it is not small. For example, the mismatch between the lattice constants of GaAs and InAs is 7.2% or 6.7% with respect to GaAs or InAs.

5. The symmetry is taken to be $\bar{4}3m$ for the piezoelectric effect. This excludes hexagonal semiconductors like GaN.

We shall first consider the elastic and piezoelectric fields of a spherical dot, since the important results follow from this.

II. ELASTIC FIELD AROUND A SPHERICAL DOT

Construct a spherical InAs dot of radius $a$ immersed in an infinite region of GaAs by the following standard sequence.\textsuperscript{17}

1. Start with an infinite sample of GaAs and remove the sphere of radius $a$ that will form the dot.

2. Transmute this material to InAs in a stress-free environment. It expands by a fraction $\varepsilon_0$ given by the difference in lattice constant, so $\varepsilon_0 = a_{\text{InAs}}/a_{\text{GaAs}} - 1 \approx 7.2\%$.

3. Apply hydrostatic pressure to reduce the volume of the dot to its original value. This gives a dilation of $\delta_{\text{com}} = -3\varepsilon_0$.

4. Put the InAs back into its cavity and allow it to relax, which causes a radial displacement $u_r(r)$ to lower the elastic energy.

The displacement after relaxation follows from Lamé’s formulas for spheres under pressure\textsuperscript{18} and is given by

$$\frac{u_r(r)}{u_r(a)} = \begin{cases} (r/a) & \text{for } r \leq a \\ (a/r)^2 & \text{for } r \geq a. \end{cases}$$

(1)

The boundary between the dot and surroundings is displaced outward by $u(a) = \frac{1}{2} \varepsilon_0 a (1 + \nu)/(1 - \nu)$. Poisson’s ratio is around $\frac{1}{3}$ for GaAs so the dot recovers about $\frac{2}{3}$ of the radius that it lost in being compressed to fit into the cavity.

The relaxation of the dot is purely hydrostatic with no shear. Its dilation, both from relaxation and the total value including the prior compression, is given by

$$\delta_{\text{rel}} = \frac{1 + \nu}{1 - \nu} \varepsilon_0,$$

(2)

$$\delta_{\text{tot}} = \delta_{\text{com}} + \delta_{\text{rel}} = -2 \frac{1 - 2\nu}{1 - \nu} \varepsilon_0.$$  

(3)
There is no dilation outside the dot. The material is compressed radially, as expected, but this is balanced by tangential extension to give no change in net volume of a shell, although it is displaced outward. Further details of this solution, and the corresponding results for slabs and cylinders, are discussed by Grundmann et al.\textsuperscript{12}

The deformation potential follows immediately from this result. For electrons there is a uniform shift of the conduction band within the dot proportional to $\delta^{tot}$, and no effect outside. The valence band is shifted rigidly by the constant dilation inside with no splitting of the bands by strain (they are split by the confinement, of course). Outside the dot, the light and heavy holes are split by the deviations of strain from a purely hydrostatic form.

III. PIEZOELECTRIC FIELD AROUND A SPHERICAL DOT

Strain induces a piezoelectric polarization $P_i = e_{ijk} \varepsilon_{jk}$. The elements of the piezoelectric tensor $e_{ijk}$ in crystallographic axes vanish unless $\{ijk\} = \{123\}$ or permutations, with $e_{123} = e_{14}$ where $e_{14}$ is the conventional piezoelectric constant.\textsuperscript{19} The polarization vanishes inside the dot because hydrostatic distortion does not cause a piezoelectric effect in a material with 43m symmetry. Thus there is no piezoelectric potential within a spherical dot.

The polarization outside the dot can be replaced by a volume charge density $\rho = -\text{div} \mathbf{P}$, which gives

$$\rho(r) = -30e_{14} \frac{1 + v}{1 - v} \varepsilon_0 a^3 \frac{xyz}{r^7}. \quad (4)$$

There is also a charge density on the surface of the dot at $|r| = a$ given by $\sigma = \mathbf{P} \cdot \hat{n}$,

$$\sigma = 6e_{14} \frac{1 + v}{1 - v} \varepsilon_0 \frac{xyz}{a^3}. \quad (5)$$

These charge generates a potential outside the dot of

$$\varphi(r) = -\frac{3e_{14} \varepsilon_0 a}{\varepsilon_r \varepsilon_0} \frac{1 + v}{1 - v} \left( \frac{a}{r} \right)^2 \left[ 1 - \left( \frac{a}{r} \right)^2 \right] \frac{xyz}{r^3}. \quad (6)$$

This is plotted in Fig. 1 and shows the expected “xyz” symmetry for 43m.

To estimate the piezoelectric potential put\textsuperscript{20} $e_{14} = -0.16 \text{ C m}^{-2}$, $\varepsilon_0 = 7.2\%$, $a = 6 \text{ nm}$, $\varepsilon_r = 13$, and $v = 0.31$. The maximum potential from Eq. (6) is then about 0.17 V at $r = a\sqrt{2}$. No screening has been included except for the background dielectric constant $\varepsilon_r$ of the semiconductor.

For comparison, the deformation potential shifts the energy of electrons inside the dot by about 0.37 eV, using a deformation potential of $-5.1 \text{ eV}$ for InAs. Thus the piezoelectric potential is unlikely to have a large effect even in a less symmetric dot where it penetrates inside. This contrasts with the potential generated by strain from gates on the surface of a semiconductor\textsuperscript{10,21} where the piezoelectric effect usually dominates. The main reason for this difference\textsuperscript{12} is that the piezoelectric potential contains an additional factor of length. Gates are typically ten times as big as a dot and therefore generate a larger piezoelectric potential.

IV. ELASTIC FIELD AROUND ANY DOT

Superposition can be used to extend the results of Sec. II to a dot of arbitrary shape and composition. This shows immediately that the dilation is proportional to the local composition; Eqs. (2)

$$\varepsilon(r) = \frac{1 + v}{1 - v} \left( \frac{a}{r} \right)^2 \left[ 1 - \left( \frac{a}{r} \right)^2 \right] \frac{xyz}{r^3}. \quad (6)$$
FIG. 1: Piezoelectric potential in the (110) plane generated by (a) spherical, (b) cubic and (c) pyramidal dots containing the same volume of InAs in GaAs. The pyramid has $a = b = h = 6 \text{ nm}$ and the potential goes from 0 (white) to $\pm 0.16 \text{ V}$ (black).

and (3) hold at each point in space. The dilation vanishes outside a dot and is constant within a dot of constant composition. The deformation potential for electrons is therefore trivial to find, but all elements of the strain tensor are needed to describe splitting of the valence bands.

A. Analogy with electrostatics

The displacement $\mathbf{u}$ during relaxation described by Eq. (1) is the same as the electric field produced by a sphere of uniform charge density and can be described by a scalar potential in the same way. The Lamé displacement potential is defined by $\mathbf{u} = \nabla \chi$ (a factor of $2G$ is often inserted but serves no purpose for this problem) and here it obeys the Poisson equation

$$\nabla^2 \chi(\mathbf{r}) = \frac{1 + \nu}{1 - \nu} \epsilon_0(\mathbf{r}) = \delta^{\text{rel}}(\mathbf{r}). \tag{7}$$

This can be solved by integration with the usual Green function to give the potential,

$$\chi(\mathbf{r}) = -\frac{1 + \nu}{1 - \nu} \int \frac{\epsilon_0(\mathbf{r}')d^3\mathbf{r}'}{4\pi|\mathbf{r} - \mathbf{r}'|}. \tag{8}$$

Expressions for the displacement and strain can be derived by taking gradients of this. The compression of $-\epsilon_0(\mathbf{r})$ must be added to the tensile strains inside the quantum dot to get the total solution; no correction is needed for the shear strains.
These considerations show that the displacement is like an electric field, with the local lattice mismatch playing the role of charge density. The elastic problem can be solved simply by the use of Poisson’s equation, rather than the biharmonic equations needed in general. It also provides a familiar way to visualize the displacement field in and around a dot. The equivalent of a point charge in electrostatics is known as a center of dilation and is widely used\textsuperscript{22} in the theory of crystal defects.

B. Expression as integrals over the surface of the dot

Starting from Eshelby’s celebrated results\textsuperscript{13} for an ellipsoidal inclusion, Downes \textit{et al.}\textsuperscript{14,15} reduced the problem of calculating the strain to integrals over the surface of a dot of constant lattice mismatch $\varepsilon_0$. Their approach can also be applied to the potential and displacement. For example, the function $1/|\mathbf{r} - \mathbf{r}'|$ in the potential (Eq. 8) can be written as $-\frac{1}{2} \text{div}'(\mathbf{r} - \mathbf{r}')/|\mathbf{r} - \mathbf{r}'|$. The divergence theorem then allows Eq. (8) and its derivatives to be written as integrals over the surface of the dot,

\begin{equation}
\chi(\mathbf{r}) = \frac{\varepsilon_0}{8\pi} \frac{1 + \nu}{1 - \nu} \int \frac{(\mathbf{r} - \mathbf{r}') \cdot dS'}{|\mathbf{r} - \mathbf{r}'|},
\end{equation}

\begin{equation}
\mathbf{u}(\mathbf{r}) = \frac{\varepsilon_0}{4\pi} \frac{1 + \nu}{1 - \nu} \int \frac{dS'}{|\mathbf{r} - \mathbf{r}'|},
\end{equation}

\begin{equation}
\varepsilon_{ij}^{\text{rel}}(\mathbf{r}) = -\frac{\varepsilon_0}{4\pi} \frac{1 + \nu}{1 - \nu} \int \frac{(x_i - x'_i)dS'_j}{|\mathbf{r} - \mathbf{r}'|^3}.
\end{equation}

The expressions are not unique because any solenoidal field can be added to the integrands, and this freedom has been used to simplify them. The strain can easily be written in a more symmetrical form if desired. Eq. (11) was given by Downes \textit{et al.}\textsuperscript{15} They further pointed out that the tensile elements of the strain can be interpreted as solid angles for a cuboidal dot, and give explicit expressions for $\sigma_{ij}$. To make contact with their result take the trace of Eq. (11), which gives

\begin{equation}
\delta_{\text{rel}} = \frac{\varepsilon_0}{4\pi} \frac{1 + \nu}{1 - \nu} \int \frac{(\mathbf{r}' - \mathbf{r}) \cdot dS'}{|\mathbf{r}' - \mathbf{r}'|^3}.
\end{equation}

The integral is the solid angle subtended at the point $\mathbf{r}$ by the surface of integration. This is $4\pi$ inside the dot and zero outside, so the result is consistent with Eq. (2).

C. Direct derivation of surface integrals

The integrals over the surface can be derived directly from the force exerted by the dot on its surroundings, which makes the transformation look less artificial. The force per unit volume is given in general by $\mathbf{K} = -\text{div}\ \mathbf{\sigma}$, which becomes

\begin{equation}
\mathbf{K} = -2G \frac{1 - \nu}{1 - 2\nu} \text{grad} \nabla^2 \chi = -2G \frac{1 + \nu}{1 - 2\nu} \text{grad} \varepsilon_0
\end{equation}

where $G$ is the shear modulus. This only describes the relaxation and is not the full force exerted by the dot on its surroundings. An elementary force $d\mathbf{P} = 2G\varepsilon_0[(1 + \nu)/(1 - 2\nu)]d\mathbf{S}$ therefore
acts outward at each point of the boundary of a dot of constant mismatch. The effect of such a force is the Kelvin problem,\(^1\) whose solution shows that a force \(\mathbf{F}\) at the origin gives displacement

\[
\mathbf{u}(\mathbf{r}) = \frac{1}{16\pi G (1 - \nu)} \left[ (3 - 4\nu) \frac{\mathbf{F}}{r} + \frac{(\mathbf{r} \cdot \mathbf{F}) \mathbf{r}}{r^3} \right].
\]  

(14)

Integration of this result over the surface of the dot yields

\[
\mathbf{u}(\mathbf{r}) = \frac{\varepsilon_0(1 + \nu)}{8\pi(1 - \nu)(1 - 2\nu)} \times \oint \left[ (3 - 4\nu) \frac{dS'}{|\mathbf{r} - \mathbf{r}'|} + \frac{(\mathbf{r} - \mathbf{r}')[(\mathbf{r} - \mathbf{r}') \cdot dS']}{|\mathbf{r} - \mathbf{r}'|^3} \right].
\]  

(15)

The difference between this integrand and that in Eq. (10) is the divergence of a solenoidal function so the surface integrals are identical. Although more clumsy, Eq. (15) has the advantage of a direct physical interpretation. Similar volume integrals and expressions for the strain can also be derived.

\section*{D. Analogy with thermoelasticity}

An alternative approach leads to the Poisson equation (7) directly from the standard elastic equations. The process of transmuting GaAs into InAs is essentially the same as a local thermal expansion, a trick that has been used in numerical work.\(^2\) Replacement of the linear expansion \(\alpha T\) by \(\varepsilon_0\) in the standard condition for equilibrium with a nonuniform temperature\(^3\) gives

\[
\text{grad} \, \text{div} \mathbf{u} - \frac{1 - 2\nu}{2(1 - \nu)} \text{curl} \, \text{curl} \mathbf{u} = \frac{1 + \nu}{1 - \nu} \text{grad} \varepsilon_0.
\]  

(16)

Substitution of \(\mathbf{u} = \text{grad} \chi\) into this leads immediately to Poisson’s equation. The behavior of the dilation \(\delta_{\text{rel}} = \text{div} \mathbf{u}\) due to the relaxation (Eq. 2) also follows trivially.

This thermoelastic equation is thoroughly analyzed in engineering textbooks\(^4\) and the integral solution (8) was given long ago in this context.\(^5\) A wide range of solutions to thermoelastic problems is available and may be applied to quantum dots. These include the following.

- Elastic field of quantum wires with rectangular and elliptic cross-sections.\(^6\)
- Elastic field of a quantum dot in the shape of a rectangular parallelepiped.\(^7\)
- Elastic field around an ellipsoid of revolution,\(^8\) including the case of different elastic constants inside and outside.\(^9\) An oblate ellipsoid may be a useful approximation to a quantum dot. The strains inside are tensile along the principal axes, generalizing the result for a sphere. Thus there is no piezoelectric charge inside an ellipsoid aligned to the crystallographic axes.

- Displacement of the free surface due to an arbitrary quantum dot buried in a semi-infinite medium.\(^10\)
- General solution for the elastic field due to an arbitrary quantum dot buried in a semi-infinite medium.\(^11\) This is derived from the displacement potential in an infinite body by an extension of the method of images, with explicit results for a spherical dot.

The relation between tensile stress and strain when the temperature varies in space is \(\sigma_{xx}(\mathbf{r}) - \nu[\sigma_{yy}(\mathbf{r}) + \sigma_{zz}(\mathbf{r})] = E[\varepsilon_{xx}^{\text{rel}}(\mathbf{r}) - \varepsilon_0(\mathbf{r})] = E\varepsilon_{xx}(\mathbf{r})\) with equivalent relations in \(x\) and \(y\). This is a reminder that the total strain \(\varepsilon_{xx}\) must to used to derive the stress, not just the part \(\varepsilon_{xx}^{\text{rel}}\) from relaxation.
V. PIEZOELECTRIC FIELD AROUND ANY DOT

The piezoelectric charge density is given in terms of the strain potential by 
\[ \rho = -e_{ijk} \partial_i \partial_j \partial_k \chi. \]
The piezoelectric potential \( \varphi \) then follows from \( \nabla^2 \varphi = -\rho/\varepsilon_0 \varepsilon_r \). These can be combined with the Poisson equation (7) for \( \chi \) to give a biharmonic equation for \( \varphi \),

\[ \nabla^4 \varphi = \frac{e_{ijk} \partial_i \partial_j \partial_k}{\varepsilon_0 \varepsilon_r} \nabla^2 \chi = \frac{1 + \nu}{1 - \nu} \frac{e_{ijk} \partial_i \partial_j \partial_k}{\varepsilon_0 \varepsilon_r} \varepsilon_0(\mathbf{r}). \]  

(17)

To find a general solution, first define a “piezoelectric pseudopotential” \( \Phi \) by

\[ \nabla^4 \Phi = \frac{1 + \nu}{1 - \nu} \varepsilon_0(\mathbf{r}). \]  

(18)

The electrostatic potential is then given by \( \varphi = e_{ijk} \partial_i \partial_j \partial_k \Phi/\varepsilon_0 \varepsilon_r \). The general solution to the biharmonic equation (18) is

\[ \Phi(\mathbf{r}) = -\frac{1}{8\pi} \frac{1 + \nu}{1 - \nu} \int \frac{\mid \mathbf{r} - \mathbf{r}' \mid \varepsilon_0(\mathbf{r}') d^3 \mathbf{r}'}{\mid \mathbf{r} - \mathbf{r}' \mid^5}, \]  

(19)

\[ \Phi(\mathbf{r}) = \frac{\varepsilon_0}{32\pi} \frac{1 + \nu}{1 - \nu} \oint \frac{\mid \mathbf{r} - \mathbf{r}' \mid (\mathbf{r} - \mathbf{r}') \cdot d\mathbf{S}'. \]  

(20)

The surface integral is for a dot of constant composition. The resulting piezoelectric potential is

\[ \varphi(\mathbf{r}) = -\frac{9e_{14}}{4\pi \varepsilon_0 \varepsilon_r} \frac{1 + \nu}{1 - \nu} \int \frac{(x-x')(y-y')(z-z')\varepsilon_0(\mathbf{r}') d^3 \mathbf{r}'}{\mid \mathbf{r} - \mathbf{r}' \mid^5}, \]  

(21)

\[ \varphi(\mathbf{r}) = \frac{3e_{14} F_z}{32\pi \varepsilon_0 \varepsilon_r G(1 - \nu)} \frac{xy}{r^3} \left[ (5 - 8\nu) + 9\frac{z^2}{r^2} \right]. \]  

(23)

Another expression for the piezoelectric potential can be obtained by integrating this potential over the surface of the dot. The result is a mixture of the surface integrals just given. Although it is more complicated, it has a direct physical interpretation and Eq. (23) provides a helpful guide to the form of potential expected around a dot.
VI. CUBOIDAL AND PYRAMIDAL DOTS

Consider cuboidal and pyramidal dots as further examples. The elastic field inside a cuboidal dot has been given before.\textsuperscript{15,24} It has a shear strain inside, unlike the sphere, and therefore the piezoelectric charge extends inside as well as outside. Let the dot have dimensions $2a \times 2b \times 2c$ with its faces normal to the crystal axes. A constant pressure acts outward along each face. The “$xy$” symmetry of the potential from a Kelvin force (Eq. 23) means that the piezoelectric effect of nearby forces on each face tends to cancel except at the corners. This results in a charge and potential with spherical symmetry around each vertex of the cube, which sum to

$$
\rho = -\frac{3\varepsilon_{14}\varepsilon_0}{2\pi} \frac{1 + \nu}{1 - \nu} \sum (-1)^n \frac{1}{R},
$$

(24)

$$
\varphi = \frac{3\varepsilon_{14}\varepsilon_0}{4\pi \varepsilon_0\varepsilon_r} \frac{1 + \nu}{1 - \nu} \sum (-1)^n R.
$$

(25)

Here $R = \sqrt{(x \pm a)^2 + (y \pm b)^2 + (z \pm c)^2}$ is the distance to each vertex and $n$ is the number of plus signs in this expression, which is summed over all vertices. The charge and potential change sign on adjacent corners to respect the simplifications made in the present work. The numerical result for the dilation was nearly constant inside the dot and zero outside, in agreement with Eq. (3).
FIG. 2: Strain as a function of $z$ for a pyramidal quantum dot with $a = b = h = 6$ nm and lattice mismatch $\varepsilon_0 = 7.2\%$ inside. (a) Dilation $\delta$ and deviation $B$ of strain from purely hydrostatic form on axis of pyramid. (b) Individual strains on axis of pyramid. (c) Individual strains on a line through $x = 3$ nm and $y = 0$, which cuts the sloping face of the pyramid at $z = 3$ nm.

The discontinuities in strain at the boundaries of the dot can be calculated immediately in the simple model used here. Consider the change in strain across the base of the pyramid. Both $\varepsilon_{xx}^{\text{rel}}$ and $\varepsilon_{yy}^{\text{rel}}$ must be continuous so $\Delta \varepsilon_{zz}^{\text{rel}} = \delta^{\text{rel}}$ to account for the change in dilation during relaxation. A further change $-\varepsilon_0$ due to the initial compression must then be added to all three tensile strains. For $\nu = \frac{1}{3}$ this leads to $-\Delta \varepsilon_{xx} = -\Delta \varepsilon_{xx} = \Delta \varepsilon_{xx} = \varepsilon_0$. The same arguments can be applied
to the point where line $B$ cuts the sloping face of the pyramid by rotating the strain tensor. An odd feature is that no discontinuity is seen in $\varepsilon_{xx}$ or $\varepsilon_{zz}$ plotted in Fig. 2(c). For $\nu = \frac{1}{3}$ and this shape of pyramid there is a cancellation at this interface between the discontinuities in strain due to the initial compression and subsequent relaxation. The numerical calculation shows only a slight discontinuity.

One route to the piezoelectric potential is the variant of Eq. (21) with $(y - y')(z - z')dS_y'$ because we need integrate over only two faces of the pyramid. It is more illuminating to build up the pyramid in thin layers parallel to its base. Reduce the height $2c$ of the cuboid to an infinitesimal thickness $\delta z$. Eqs. (24) and (25) then show that the charge and potential around the corner at $a, b, 0$ of a rectangular lamina in the plane $z = 0$ are

$$\rho = -\frac{3e_{14} \varepsilon_0 \delta z}{2\pi} \frac{1 + v}{1 - v} \frac{z}{R^3},$$

$$\varphi = -\frac{3e_{14} \varepsilon_0 \delta z}{4\pi \varepsilon_0 \varepsilon_r} \frac{1 + v}{1 - v} \frac{z}{R},$$

where $R = \sqrt{(x - a)^2 + (y - b)^2 + z^2}$. The other vertices have similar expressions and the sign alternates on adjacent vertices. This can be integrated up the sloping edge of the pyramid from $(a, b, 0)$ to $(0, 0, h)$. The charge density from the corner of the lamina has the same form as the electrostatic potential from a dipole oriented along $z$, and the pyramid therefore has lobes above and below the four edges whose sum cancels near the top of the pyramid. This was seen in the numerical work (Ref. 12, Fig. 8). The potential from the edge between $(a, b, 0)$ and $(0, 0, h)$ is

$$\varphi^{(++)} = -\frac{3e_{14} \varepsilon_0}{4\pi \varepsilon_0 \varepsilon_r} \frac{1 + v}{1 - v} \frac{h^2}{L} \left[ \frac{R_{++}}{L} \right] + \frac{a(x - az/h) + b(y - bzh/h)}{L^2} \ln \frac{R_{++} + R_h + L}{R_{++} - R_h - L}.$$

Here $L = \sqrt{a^2 + b^2 + h^2}$, the length of a sloping edge of the pyramid; $R_{++} = \sqrt{(x - a)^2 + (y - b)^2 + z^2}$, the distance to the corner of the base at $(a, b, 0)$; and $R_h = \sqrt{a^2 + y^2 + (z - h)^2}$, the distance to the peak of the pyramid. The divergence in the logarithm on the sloping edges of the pyramid is suppressed by the prefactor. The other three edges give similar contributions with opposite signs from alternate edges.

The piezoelectric potential from a sphere, cube and pyramid are plotted in Fig. 1 for a section through the axis of the dots in the $(110)$ plane. The pyramid has $a = b = h = 6 \text{ nm}$ and the other dots have the same volume, which permits a common scale of $\pm 0.16 \text{ V}$. The potential reaches about $\pm 90 \text{ mV}$ for the pyramid. Its lower symmetry allows the potential to penetrate inside more strongly but the main effect is near the corners in the basal plane where the wavefunction is weak. The piezoelectric potential is therefore likely to have only a weak influence on the energy levels.

This calculation has used $e_{14}$ for GaAs everywhere. The piezoelectric constant for InAs is considerably smaller and this will reduce the polarization charge inside the dot. However, the discontinuity in $\mathbf{P}$ will then induce charge on the surface of the dot so the overall change is reduced. (It would make no difference at all for a spherical dot.)

VII. CUBIC ELASTIC BEHAVIOR

The above calculations have used an isotropic approximation for the elastic behavior of the semiconductor. Unfortunately this is not particularly accurate as the anisotropy ratio $(c_{11} - c_{12})/2c_{44} \approx
0.55 for GaAs. We shall therefore look briefly at improved approaches.

The $x$-component of the thermoelastic equation (16) for cubic symmetry becomes

\[
\begin{align*}
(c_{12} + 2c_{44})\frac{\partial}{\partial x} \text{div} \mathbf{u} - c_{44}(\text{curl curl} \mathbf{u})_x \\
+ (c_{11} - c_{12} - 2c_{44})\frac{\partial^2 u_x}{\partial x^2} = (c_{11} + 2c_{12})\frac{\partial}{\partial x}\varepsilon_0,
\end{align*}
\]

(31)

with similar equations in $y$ and $z$. Taking the divergence shows that the dilation no longer obeys Poisson’s equation. A single scalar potential cannot be used, but the equation has been solved\(^3\) by using a separate scalar potential for each component of $\mathbf{u}$ and taking a Fourier transform. Unfortunately the results are not simple for a cubic material. The distortion around a center of dilation in a cubic material has been studied in connection with lattice defects\(^3\) but again the results are complicated. The dilation no longer vanishes but is positive along some directions and negative along others.

As the treatment of cubic symmetry appears complicated, we would like to continue to use the simple results for an isotropic medium with an appropriate value for Poisson’s ratio $\nu$. Often one sets $\nu = c_{12}/(c_{11} + c_{12}) \approx 0.31$ which is appropriate for strain in a (100) plane. Another common choice is $\nu = c_{12}/2(c_{12} + c_{44}) \approx 0.24$, which is considerably different. A prescription is clearly needed.

The most crude approach is simply to drop the awkward terms like $\frac{\partial^2 u_x}{\partial x^2}$ from Eq. (31). The resulting Poisson equation has a very low effective value for Poisson’s ratio of

\[
v_{\text{eff}} = \frac{c_{11} + c_{12} - 2c_{44}}{c_{11} + 3c_{12} + 2c_{44}} \approx 0.14.
\]

(32)

A next step is to substitute the simple scalar potential $\mathbf{u} = \text{grad} \chi$ into Eq. (31). Integration with respect to $x$ yields

\[
(c_{12} + 2c_{44})\nabla^2 \chi + (c_{11} - c_{12} - 2c_{44})\frac{\partial^2 \chi}{\partial x^2} = (c_{11} + 2c_{12})\varepsilon_0.
\]

(33)

Adding the similar equations with $y$ and $z$ gives another Poisson equation, as desired, with

\[
v_{\text{eff}} = \frac{c_{11} + 2c_{12} - 2c_{44}}{2(c_{11} + 2c_{12} + c_{44})} \approx 0.19.
\]

(34)

Again this is lower than either of the values written down initially.

A more rigorous approach draws on the theory of inclusions in anisotropic media.\(^3\) This shows that the strain is uniform inside an ellipsoidal quantum dot even if its elastic constants are different from those of the surroundings.\(^3\)\(^4\)\(^5\) The strain can be calculated by successive approximations\(^4\)\(^5\) or by integration.\(^6\) The effective value of $\nu$ in the isotropic approximation could then be chosen so that the dilation inside the dot is correct. This approach gives $v_{\text{eff}} = 0.25$ for a spherical dot, using the elastic constants of GaAs everywhere.

It might be expected that this value of $\nu$ would improve further the agreement between the simple calculations presented in Sec. VI and the numerical work,\(^1\) but this is not the case. For example, the negative dilation inside the dot is predicted to be 9.7% using $\nu = 0.25$ but the computed value was 7.5–8.0%. This may indicate that $v_{\text{eff}}$ depends strongly on the shape of the dot. A very flat ellipsoidal dot, for example, responds in the same way as a slab\(^3\)\(^4\)\(^5\) and gives $\nu \approx 0.31$ for a slab normal to a cubic axis. It is clearly difficult to allow for cubic anisotropy in the analytical approach, and this sets a limit to the accuracy of the simple method.

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VIII. CONCLUSIONS

The elastic field of a quantum dot buried in an infinite isotropic medium can be solved using a scalar potential. The dilation is a local function of the lattice mismatch and provides the charge density in Poisson’s equation for the elastic potential. The deformation potential for electrons in a $\Gamma$ valley is therefore constant inside a dot and vanishes outside. Holes or a multi-valley conduction band (as in Si or Ge) are more complicated because the bands are split by the individual components of the strain. The displacement is analogous to the electric field, which provides a simple way to visualize the elastic field. The standard techniques for solving electrostatic problems can be used. For example, the effect of the elastic field from a dot on a nearby quantum well could be modelled with a few multipole moments. Efficient numerical methods are also available for the solution of Poisson’s equation. Other profitable analogies are with thermoelasticity and inclusions, with numerous helpful solutions available.

The piezoelectric potential can be calculated from an integral over the surface of the dot, and can be visualized using the potential generated by elementary forces on its surface. The small size of a typical dot reduces the magnitude of the potential below the deformation potential and band offsets. Nevertheless it may be significant because it is the only potential seen by electrons outside, where the deformation potential vanishes, and may modify the capture of carriers. It also breaks the symmetry inside but this effect is small because the piezoelectric potential is large only in the extremities of the dot.

It has been assumed that the elastic properties are homogeneous and isotropic, but comparison is encouraging with numerical results that did not make this approximation. The methods presented here for solving the elastic field around a dot, requiring only the solution of Poisson’s equation, should therefore be of wide applicability. One application is to a strained quantum well with imperfect interfaces, where randomness in the elastic field contributes to interface roughness scattering. The deformation potential has been calculated for electrons in Si:Ge alloys\textsuperscript{37} and there should also be a piezoelectric effect in III–V materials.

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\begin{itemize}
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22. C. Teodosiu, Elastic models of crystal defects (Springer-Verlag, Berlin, 1982).
26. Ref. 17, Sec. 162.
27. Ref. 24, sec. II.2; a simple interpretation is given in Ref. 15.
30. Ref. 17, Sec. 156.