Strain Relaxation in Semiconductor Devices

by

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Abstract

Strained layers are incorporated into many electronic devices and particularly into semiconductor lasers. These strained layers can relax, both elastically and plastically, which often impairs the performance of the device.

This thesis presents several methods for calculating elastic strain relaxation: a Fourier-series method for stresses imposed on the surfaces of a rectangular block; a Fourier-integral for stress imposed on the surfaces of an infinite layer; and a Green-function method for the stress field about buried inclusions. The methods are used to calculate the strain distributions in a transmission electron microscopy sample, the relaxation at the end facet of a strained-layer laser, and the strain field about a rectangular buried layer. The effects of the strain relaxation on the optical absorption of the laser facet and the zone-centre band structure of the buried layer are discussed.

The equilibrium theory of critical thickness is examined in detail and is shown to make unreasonable predictions for highly strained layers; a modification which corrects this behaviour is suggested. The equilibrium theory equates the line tension of a strain relieving dislocation to the strain energy it relieves in the layer. The additional energy corrections which can be included in the line tension are discussed, together with the failure of the equilibrium theories to reliably predict plastic relaxation in all situations.
Acknowledgements

Arriving in cosmopolitan Guildford was a daunting experience for one, like myself, from such a provincial county as Norfolk. I am therefore indebted to all the long established locals who made the transition as smooth as it was.

During my time in Guildford, a great many new friends have come my way. To thank all of them individually would use more rain forest then the rest of this thesis, therefore I hope they will understand if I decline to do so. However, some people are worthy of a particular mention.

Dave Faux, together with Dave Dunstan and Eoin O’Reilly, has provided suitable guidance (and travelling funds) through the last three years. The occupants\(^1\) of office three have always been there when I needed someone to talk to, and sometimes when I did not. Steve is thanked for guiding me through DM’s entertaining network and, likewise, Herbert’s lessons on the use of the piles of microchips are appreciated. A certain Scotsman should be acknowledged for some dodgy data and some that was not so dodgy.

On a more personal note . . .

Filomena, you have given me a great deal. Thankyou.

Finally, for this, and for my siblings, you must blame my parents, and for my parents you must congratulate my grandparents, to whom I dedicate this thesis.

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\(^1\)The use of the word ‘colleagues’, or perhaps even ‘humans’ would not be appropriate here. Although, of course, ‘friends’ would.
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Chapter 1

Introduction

Strained-layer semiconductor structures are commercially produced in vast numbers creating a multi-million pound annual turnover. They find application principally in the semiconductor laser, which is used in the communications industry and in optical data storage. The vast expansion in the semiconductor laser industry occurred during the late seventies and eighties; long after the first semiconductor lasers were produced by three different groups in 1962. In the early days there was a major problem with the reliability of the devices. Lasers could be produced that worked well at low temperatures, but when these devices were operated at room temperatures their lifetimes were too short for commercial exploitation. Low reliability, caused by the exceptionally high rate of stimulated emission and insufficient dissipation of the heat generated, has always been the bugbear of the semiconductor laser. The first useful devices followed the introduction of the heterostructure in 1969.

A heterostructure uses different materials with suitable band-gaps and refractive indices to confine, both electronically and optically, the lasing action to a small region, known as the active region, within the device. The heterostructure laser has several advantages over homostructure devices, but there are also drawbacks: the interface between two different materials (the heterojunction) involves the joining of materials with potentially different lattice parameters. The first heterostructures used GaAs/GaAsP and failed because the lattice mismatch resulted in too many defects at the interfaces. Consequent development
continued with lattice matched GaAs/AlGaAs heterostructures, resulting in commercial
devices in 1971. Vast numbers of lattice-matched devices were designed and implemented
until improved fabrication techniques allowed the introduction of strain.

By the early eighties, crystal growers could produce high quality interfaces between
incoherent materials; a result of efforts to increase the range of materials available to
device designers. This, together with the realisation, by Adams (1986), that strain may
advantageously alter the electronic and optical properties of materials, resulted in the
appearance of strained-layer lasers. To date, development has concentrated on strained
layers. Meanwhile, work to improve their efficiency, reliability, power, wavelength range,
etc. is continuing.

Strain is incorporated into a device to improve many of its properties, but strained
layers are prone to degradation [Jain and Hayes(1991) and Fitzgerald (1991)]. Material in
a strained state will always tend to relax, usually with the introduction of dislocations into
the structure. It is unfortunate that these dislocations, and their subsequent propagation,
reduce the lifetime of many lasers.

1.1 Laser degradation

After the failure of many early attempts to produce reliable lasers, researchers began to
believe this limitation was intrinsic to semiconductor lasers. They were relieved when
Hartman and Hartman (1973) discovered that dislocations were the main cause of rapid
laser degradation. The degradation of the early heterostructures was associated with the
formation of long regions of zero luminescence within the active layer. These are now
known as dark-line defects and after examination by transmission electron microscopy
they have been shown to be a disordered network of dislocations [Petroff and Hartman
(1973)]. There is evidence to show that dark-line defects grow from a single dislocation
which threads through the heterostructure layers during growth, and subsequently grows
and multiplies in the plane of the structure.

These dislocation networks introduce considerable non-radiative recombination, which
increases the threshold current-density and decreases the efficiency. A dark-line defect, or several, may grow to such an extent that the laser will cease to operate altogether. Study by Petroff et al. (1974) has shown that dark-line defects grow in the presence of recombining holes and electrons. A dislocation acts as a recombination centre and so its surroundings heat up during laser operation; this energy can then create more defects and thus follows the growth of a dark-line defect.

Progress is made by eliminating these dislocations for which three sources have been identified: threaders from the substrate, dislocations created at layer interfaces and those introduced after growth by handling and attaching contacts. By choosing suitable substrates and optimising epitaxial growth, AlGaAs lasers with appreciable lifetimes can be produced. Another material suitable for lasing, InP, has proved to be inherently more resistant to defect formation. This resistance arises because: (a) InP has a lower band gap which gives less energy per recombination event; and (b) Indium and phosphorous atoms have considerably different atomic radii, which can cause pinning of dislocations.

Laser degradation is now split into three categories [Bangert (1994)]: rapid degradation arising from the growth of dark-line defects, where the dislocations act as recombination centres and the recombination enhances dislocation glide and climb; gradual degradation is the precipitation of point defects and dislocation loops, which are again enhanced by non-radiative recombination; and catastrophic failure which involves damage at the end facets, and can occur in the absence of defects. Principally these classifications apply to AlGaAs lasers but modern InGaAsP based lasers also degrade, albeit at a somewhat slower rate.

The degradation of a device, especially a laser, is closely linked to the defects and the way in which they nucleate and move, which is turn related to the strain distribution within the device [Hartman and Hartman (1973)]. Strain can also directly influence the band structure of a device [O’Reilly (1989)]. Material under compressive strain has an increased bandgap and that under tensile strain has a decreased bandgap. Therefore, when the strain in a particular region of a device relaxes, there may be a detrimental change in the electronic properties of the device. For these reasons, knowledge of the strain field in
strained-layer structures may prove invaluable in the understanding of device degradation.

1.2 Strain relaxation

Strain relaxation can be split into two types: elastic relaxation and plastic relaxation. Plastic relaxation occurs with the nucleation and movement of dislocations, whereas elastic relaxation is the simple relaxation one associates with a stretched rubber band contracting to its preferred shape. Importantly, elastic relaxation does not involve the motion of dislocations.

There is a large body of literature on the critical-thickness of heteroepitaxial strained-layers [Jain and Hayes (1991) and Fitzgerald (1991)], which is concerned with the plastic relaxation of strain through the introduction of misfit dislocations. Study of elastic relaxation has highlighted the strain relaxation in the form of bending of the entire structure (cf. a bimetallic strip), the bowing of material at the end facets of lasers, the relaxation during fabrication (both during epitaxy and after subsequent etching) and the relaxation of buried-layers after fabrication.

Given the atomic nature of these devices, it is surprising that most analyses have used continuum linear elasticity theory; very few have been concerned with the discrete nature of the materials. Even when dealing with plastic relaxation, which by its very nature means the material is inelastic, most models have been based on elasticity theory.

1.3 Elasticity theory

Linear elasticity is a theory of elasticity that treats only systems with very small deformations, such that the displacements of a body, which arise from an externally applied stress, do not substantially alter the action of any other stresses applied. A vast number of books have been written on linear elasticity. The book by Timoshenko and Goodier (1970) was used as reference material for this thesis, but those by Love (1944) and by Pearson (1959) are also useful.
There are three important quantities of interest in a strained body, the stresses, the strains and the displacements. The displacements can be expressed as a vector, \( u_i \), where \( i = 1, 2, 3 \), and the strains subsequently take the form of the 2\(^{nd} \) rank tensor

\[
\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \tag{1.1}
\]

Hooke’s law is the well known result that strain is proportional to stress. For a fully anisotropic material, Hooke’s law must be expressed as an equation linking two 2\(^{nd} \) rank tensors through the elastic constants, \( S_{ijkl} \),

\[
\varepsilon_{ij} = S_{ijkl} \sigma_{kl}. \tag{1.2}
\]

The fourth rank tensor \( S_{ijkl} \) has 81 elements known as the elastic compliance constants. Fortunately, through the symmetry of the stress and strain tensors and consideration of the free energy, it can be shown that only 21 of these elements are independent for an anisotropic medium [Lekhnitskii (1963)]. Their number is reduced further in most crystal structures.

The majority of semiconductors used in devices today have the zinc-blende structure. The symmetry of this crystal means that only three independent elastic constants are required. The anisotropy of the zinc-blende crystal structure is shown clearly in figure 1.1, which is a sketch of the Youngs modulus, \( E \), as a function of direction in InP. The maximum value of \( E \) is roughly \( 10^{11} \) Pa and the minimum is about \( 6 \times 10^{10} \) Pa. Such a large degree of directional difference in \( E \) would suggest that it is important to take account of the crystals anisotropy; however earlier work by Faux and Haigh (1990) has shown that the difference in the strain field calculated by assuming isotropy is only about 6%. For this reason, and because the analysis is simplified, in this thesis it will be assumed that the semiconductor materials are isotropic. The assumption means that the error in strains and stresses will be several percent.

Hooke’s law for an isotropic material is

\[
\varepsilon_{ij} = \frac{1}{E} \left[ (1 + \nu)\sigma_{ij} - \delta_{ij} \nu \sigma_{kk} \right], \tag{1.3}
\]

\(^1\)Index notation is useful in showing the multiplicity of many equations in elasticity theory. However some results are clearer if expressed in cartesians explicitly. Both notations are clearly defined in appendix A.
where, following the usual index notation, the repeated index, $k$, implies summation over $k$ and $\delta_{ij}$ is the kronecker-delta function. $E$ is, once again, Young’s modulus and $\nu$ is the Poisson’s ratio. The stresses can similarly be expressed in terms of strains,

$$\sigma_{ij} = \frac{E}{1 + \nu} \left[ \epsilon_{ij} + \delta_{ij} \frac{1}{1 - 2\nu} \epsilon_{kk} \right].$$

The equations given above relate stresses and strains in three-dimensions. If a problem can be reduced to two-dimensions, it is usually easier to solve. There are two classes of problem for which this is possible. They are known as plane stress and plane strain.

Plane stress occurs in very thin plates, shown in figure 1.2(a), loaded uniformly at the edges. Plane strain occurs in very thick objects, shown in figure 1.2(b), where the strains are zero in one direction.

<table>
<thead>
<tr>
<th>$\delta_{ij}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0$ for $i \neq j$ and $1$ for $i = j$.</td>
</tr>
</tbody>
</table>
edges and not on the faces of the plate. In this case it may be assumed that there are no
stresses with components perpendicular to the plate, and that the other components do not
vary across the thickness of the plate.

Plane strain occurs in long bodies, see figure 1.2(b), where it is assumed that if end
effects can be ignored, the strain does not vary along the axis of the body. This situation
occurs where the region being considered is far from the ends of the body.

Reducing a problem to two-dimensions allows certain stresses and strains to be set to
zero, which simplifies the stress-strain relations. Equations 1.3 can be reduced in plane
strain to

\[ \varepsilon_{ij} = \frac{1 + \nu}{E} [\sigma_{ij} - \nu \delta_{ij} \sigma_{kk}] \quad \text{for } i, j = 1, 2 \quad \text{and} \quad \sigma_{33} = \nu (\sigma_{11} + \sigma_{22}), \]  

(1.5)

and in plane stress to

\[ \varepsilon_{ij} = \frac{1}{E} [(1 + \nu) \sigma_{ij} - \nu \delta_{ij} \sigma_{kk}] \quad \text{for } i, j = 1, 2. \]  

(1.6)

As well as satisfying Hookes laws the material must also be in mechanical equilibrium.
All problems treated in this thesis will have neither net acceleration nor any body forces.
Therefore all elemental volumes inside the material must have zero net force acting upon
them. This condition yields the equilibrium equations,

\[ \frac{\partial \sigma_{ij}}{\partial x_j} = 0, \]  

(1.7)

where, once again, the repeated index indicates summation.

In plane stress and plane strain there are three strain components which are related to
only two displacement fields, u and v, which are the displacements in the x and y directions
respectively. Thus,

\[ \varepsilon_{xx} = \frac{\partial u}{\partial x}, \quad \varepsilon_{yy} = \frac{\partial v}{\partial y} \quad \text{and} \quad \varepsilon_{xy} = \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right). \]  

(1.8)

It is therefore possible to express one of the strains in terms of the other two,

\[ \frac{\partial^2 \varepsilon_{xx}}{\partial y^2} + \frac{\partial^2 \varepsilon_{yy}}{\partial x^2} = 2 \frac{\partial^2 \varepsilon_{xy}}{\partial x \partial y}. \]  

(1.9)
Equation 1.9 is known as the compatibility condition. Using equations 1.5 and 1.6 and the two-dimensional equations of equilibrium, it is possible to express the compatibility condition in terms of the stresses,

\[
\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) (\sigma_{xx} + \sigma_{yy}) = 0. \tag{1.10}
\]

A problem can be solved by finding stress fields that satisfy the equilibrium equations and the compatibility condition subject to the boundary conditions of the problem.

If the stresses are expressed as the derivatives of a function \( \Phi \) in the following manner:

\[
\sigma_{xx} = \frac{\partial^2 \Phi}{\partial y^2}, \quad \sigma_{yy} = \frac{\partial^2 \Phi}{\partial x^2} \quad \text{and} \quad \sigma_{xy} = -\frac{\partial^2 \Phi}{\partial x \partial y}, \tag{1.11}
\]

then these stresses are both solutions of the equilibrium equations and the compatibility condition if the function \( \Phi \) satisfies

\[
\frac{\partial^4 \Phi}{\partial x^4} + 2\frac{\partial^4 \Phi}{\partial x^2 \partial y^2} + \frac{\partial^4 \Phi}{\partial y^4} = \nabla^4 \Phi = 0. \tag{1.12}
\]

If this is the case then \( \Phi \) is known as an Airy stress function. A problem in two-dimensional elasticity can therefore be simplified to finding an Airy stress function, such that the stresses given by 1.11 satisfy the boundary conditions.

The strain energy stored in the body is often required and can be calculated from the stress and strain fields. When Hooke's Law and the simple force \( \times \) displacement relationship for work done are used, the following expression is obtained,

\[
E_s = \frac{1}{2} \int_V \sigma_{ij} \epsilon_{ij} dV. \tag{1.13}
\]

### 1.4 Dislocations

A number of books have been written on dislocations: Hull and Bacon (1984) give a good introduction to the topic, whereas Cottrell (1953) and Hirth and Lothe (1968) give more detail. A brief introduction to the concepts required later in this work is presented here.

The concept of the dislocation arose from the study of plastic deformation, where a crystalline material can often deform elastically only up to a limit. Beyond this limit, the
material does not relax to its original shape; it has undergone some irrecoverable or plastic deformation.

Study of single crystals showed that often one part of a crystal would slide as a unit across a neighbouring part (see figure 1.3).

![Figure 1.3: Under external force, part of a crystal can slip over an adjacent part](image)

1.4.1 Burger's vector

In order to describe slip within a crystal one needs to introduce the dislocation and Burger's vector. Figure 1.4 shows a region of crystal over which slip has occurred: the boundary, S, is known as a dislocation line, and the vector, \( \mathbf{b} \), describing the direction and magnitude of slip, is known as the Burger's vector. The Burger's vector can similarly be defined as the difference in displacement (measured in lattice spacings) obtained by completing a loop about the dislocation line and completing the same loop in a perfect crystal.

![Figure 1.4: The line S bounds a region over which slip has occurred.](image)

The Burger's vector is constant along the dislocation line, but the form of the dislocation at each point depends on the angle the Burger's vector makes to the dislocation line. At A, \( \mathbf{b} \) is perpendicular to S and the dislocation has pure edge character (shown more clearly in figure 1.5(a)), whereas at C the dislocation has pure screw character (shown in figure 1.5(b)). Around the line S the dislocation has a mixture of edge and screw character, the possible
combinations will depend on the crystal structure of the material.

![Diagram of crystal structure](image)

Figure 1.5: (a) A pure edge dislocation and (b) a pure screw dislocation.

### 1.4.2 Glide and climb

It is the motion of dislocations that causes plastic deformation. The motion can occur by either glide or climb (see figure 1.6). Glide involves a rearrangement of atomic bonds but no net movement of atoms. On the other hand, climb involves both bond rearrangement and net translation of atoms. There is considerably more resistance to the movement of atoms.

(a) Glide occurs through the rearrangement of atomic bonds. Each step in this figure involves two bonds breaking and two others forming.

![Diagram of glide](image)

(b) Atoms move in the process of climb. Each step in the figure involves a row of atoms moving one lattice spacing down the crystal.

![Diagram of climb](image)

Figure 1.6: Dislocations move through glide or climb.
than to the swapping of bonds; thus glide is kinetically more favourable than climb. This
difference has important implications for relaxation of strained-layers.

1.5 Electronic structure

The electronic properties of semiconductors are very complicated. In this section a very
brief description of some of the features, and the way strain influences them, is presented.
A more detailed and informative discussion can be found in the book by Harrison (1980)
or in several review articles including, for example, O’Reilly (1989).

It is instructive to begin by considering a free atom. For a single atom the \textit{s} electronic
orbital usually has a lower energy than the \textit{p} orbital. When many atoms are brought together
to form a crystal the outermost electrons interact. In a manner similar to the interaction
of the 1\textit{s} orbitals of two hydrogen atoms forming a hydrogen molecule, the outermost \textit{s}
and \textit{p} electrons of the atoms forming semiconductor crystals interact to produce bonding
and anti-bonding states. These states are a linear combination of the \textit{s} and \textit{p} orbitals of the
single atoms.

The bonding states are known as the conduction band and the anti-bonding states are
known as the valence band. The energy gap between the lowest \textit{s} anti-bonding state and
the highest \textit{p} bonding state is known as the band gap. The interactions of the electronic
orbitals are different for electrons with different velocities and the way in which the bands
vary with electron velocity is known as the band structure of a semiconductor. At the centre
of the Brillouin zone, the zone centre, the orbitals interact in a manner which means the
lowest energy state of the conduction band and the highest energy state of the valence band
are comprised of a linear combination of \textit{s} and \textit{p} orbitals respectively; however, at other
points in the Brillouin zone the bands are a mixture of \textit{s} and \textit{p} orbitals. Figure 1.7 illustrates
the band structure of GaAs.

The complex behaviour of most of the band structure is difficult to explain without
considering the interactions of all the bands, however the simple picture of interacting \textit{s}
and \textit{p} orbitals can be useful in understanding some basic ideas. The spin-orbit split-off

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Figure 1.7: The band structure for GaAs. The labels L, Γ, X, U and K refer to particular points on the Brillouin zone surface, and the labels A, Δ and Σ refer to particular directions in the Brillouin zone. The magnified region shows the detail at the top of the valence band.

The valence band can, at the zone centre, be explained by analogy to the spin-orbit interaction in a single atom. Under hydrostatic pressure the overlap between the orbitals increases, the interaction energies increase and therefore the band gap will increase. Under axial strain the symmetry of the p orbitals is removed and the degeneracy of the heavy-hole and light-hole bands may lift. Figure 1.8 shows how axial strain can remove the symmetry of the p orbitals. The conduction band is unaffected by axial strain because of the spherical symmetry of the s states.

The many complicated interactions between all the states, not only the outermost s and p states, has been simplified by Luttinger and Kohn (1955) to a Hamiltonian in the form of a matrix. It is now known as the Luttinger-Kohn Hamiltonian and is discussed by O’Reilly (1989). The 6 × 6 Hamiltonian includes the heavy-hole, light-hole and spin-orbit split-off band interactions. Expressed in a basis combining the spin-up and spin-down functions, ↑ and ↓, and the spatial functions, similar to the 3p state functions, X, Y and Z, it is

\[
H = \begin{bmatrix}
\alpha + l_{zz} - \Delta & m_{xy} - i\Delta & m_{xz} & 0 & 0 & \Delta \\
m_{xy} + i\Delta & \alpha + l_{yy} - \Delta & m_{yz} & 0 & 0 & -i\Delta \\
m_{xz} & m_{yz} & \alpha + l_{zz} - \Delta & -\Delta & -i\Delta & \Delta \\
0 & 0 & -\Delta & \alpha + l_{zz} - \Delta & m_{xy} + i\Delta & m_{xz} \\
0 & 0 & -i\Delta & m_{xy} - i\Delta & \alpha + l_{yy} - \Delta & m_{yz} \\
\Delta & i\Delta & 0 & m_{xz} & m_{yz} & \alpha + l_{zz} - \Delta
\end{bmatrix}
\]

(1.14)

where \( \alpha = a(\varepsilon_{zz} + \varepsilon_{yy} + \varepsilon_{xx}) \), \( l_{zz} = b(2\varepsilon_{xx} - (\varepsilon_{yy} + \varepsilon_{zz})) \), \( l_{yy} = b(2\varepsilon_{yy} - (\varepsilon_{zz} + \varepsilon_{xx})) \),
Figure 1.8: The $p$ orbitals of a crystal experiencing either no strain or hydrostatic strain are illustrated in (a). The $p$ orbitals of a crystal under axial strain are shown in (b). These two illustrations show how axial strain removes the symmetry of the $p$ orbitals but hydrostatic strain does not.

\[ l_{zz} = b(2\varepsilon_{zz} - (\varepsilon_{xx} + \varepsilon_{yy})), \quad m_{xy} = \sqrt{3}d\varepsilon_{xy}, \quad m_{yz} = \sqrt{3}d\varepsilon_{yz}, \quad m_{xz} = \sqrt{3}d\varepsilon_{xz} \quad \text{and} \quad \Delta = \frac{E_{SO}}{3}; \]

and where $a$ is the hydrostatic deformation potential, $b$ and $d$ are the (001) and (111) axial deformation potentials respectively and $E_{SO}$ is the spin-orbit splitting for zero strain. For any strain state, the eigenvalues and eigenvectors of the Hamiltonian give the energies and character of the valence band for electrons with no momentum, known as the zone centre. For mobile electrons the picture is more complicated but, because most stimulated emission in the laser devices occurs near to the zone centre, simply finding the eigenvalues of the Hamiltonian provides useful information.

Rather than expressing the Hamiltonian in the $X$, $Y$ and $Z$ basis, it is possible to choose a basis corresponding to the light-hole, heavy-hole and spin-orbit split-off bands; this results in a more simple Hamiltonian from which the energies of the bands can be deduced more easily.

The dependence of the conduction band can be included in an $8 \times 8$ Hamiltonian; however, it is simpler to use the following,

\[ E_c = E_c^0 + a_c\varepsilon_{vol} \quad \text{and} \quad E_v = E_v^0 + a_v\varepsilon_{vol}, \quad (1.15) \]
where $E_c$ is the conduction-band energy and $E_v$ is the average valence-band energy; and where $E_i^0$ are the unstrained band edges, $a_i$ are the hydrostatic deformation potentials and $\epsilon_{\text{vol}}$, equal to $\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$, is the hydrostatic strain.

The Luttinger-Kohn Hamiltonian together with equations 1.15 are used in chapter 4 when the influence of strain relaxation on the electronic properties of a buried layer is discussed.
Chapter 2

Fourier-Series Method for calculating Strain

The theory of the Fourier-series method for calculating strain distributions is described in this chapter. Section 2.1 contains a review of previous methods of determining strain and the development of the Fourier-series method is justified. In section 2.2 the theory for a single rectangular block is given, and in sections 2.3 and 2.4 the extensions required to treat several ‘linked’ blocks are discussed.

2.1 Introduction

Strain distributions can be calculated in a variety of ways. A popular and long-established method is finite-element analysis (FEA).

2.1.1 Finite-element analysis

By dividing a complicated object into a finite number of smaller and simpler elements, finite-element analysis can calculate the strain distribution of objects with complicated geometries. Commercial packages have been developed for the engineering world and these have found application to semiconductor structures.
For instance, Harvey et al. (1993) used FEA in developing a strain-measuring technique using transmission electron microscopy (TEM). The strain in a strained-layer 90°-wedge sample can be deduced from the contrast patterns of TEM. FEA was used to calculate the relaxation of the samples so that its effect on the contrast patterns could be accounted for. The relaxation of a strained buried layer was calculated using FEA by Faux et al. (1994). The layer was modelled with the ANSYS\textsuperscript{1} package by heating a system comprising of a rectangular region with a different thermal expansivity to its surroundings. Grundmann et al. (1994) used FEA to calculate the strain field of a crescent-shaped strained quantum wire, and Nishi et al. (1994) considered a triangular quantum wire. Both workers examined the influence of the relaxation on the electronic properties of the wires. Van Miegham et al. (1994) applied FEA to the relaxation of laterally small strained epilayers and Christiansen et al. (1994) studied the similar situation of strained island growth. The strains predicted by finite element analysis were compared to measurements by convergent-beam electron diffraction.

With the exception of the work by Faux et al., FEA has been applied to structures with low aspect ratios. The method involves dividing the structure into many smaller elements and the accuracy of the results depends on both the choice of a suitable set of elements and on the number of elements used. High aspect-ratio structures, like many strained-layers, require a large number of elements, which is computationally demanding. Faux et al.'s calculations for layers with aspect ratios of 40:1 required approximately 2000 elements, which was at the limits of the available computing power.

The results of FEA are not analytic, and interpolation is required to find strains away from mesh points. Functional forms are often more useful for further analysis based on the calculated strain distributions. FEA analysis is very good for treating structures with complex geometries, but strained-layer structures usually have simple geometry; therefore, even though commercial packages are available, the computational limits and lack of analytic solutions mean that other methods of strain calculation are desirable.

\textsuperscript{1}ANSYS Version .50 by Swanson Systems Inc., Johnson Road, P. O. Box 65, Houston, PA 15342-0065, U. S. A.
2.1.2 Boundary-element analysis

Boundary element analysis (BEA) is another numerical technique, described well by Banerjee (1994). Unlike FEA, by transforming a problem defined on a region to the region’s boundary, BEA requires the meshing of only the surfaces of the structure. As a result, the method is much faster and is still able to handle complicated geometries. Unfortunately there are few commercial packages available, the mathematics is difficult and the results are not analytic. Therefore the technique is not widely used by engineers, and has not been applied to semiconductor structures at all.

2.1.3 Analytic solutions

Analytic solutions are usually specific to particular problems. For strained-layer structures, relaxation at the surfaces, the curvature and stress in multilayer structures and the relaxation of buried inclusions have been considered.

Multilayers

In 1969 Saul extended the bimetallic strip analysis of Timoshenko (1925), which calculates the maximum stress in the strips, to study growth of GaP on GaAs when an intermediate layer of GaAsP was used in an effort to improve growth quality. Photoluminescence was used by Dingle and Wiegmann (1975) to examine the layer stress in AlGaAs/GaAs heterostructures shortly before Olsen and Ettenberg (1977) continued the elasticity analysis to determine the in-plane stress and bending of multilayers. Using the same analysis, Feng and Liu (1983) studied the effect of growth temperature and thermal strains on multilayer structures.

When Chu et al. (1985) studied InGaAs/InP structures using X rays to measure curvature and X-ray double-crystal diffraction to measure mismatch, he discovered that the presence of misfit dislocations was required to account for a discrepency between the value of curvature measured and the value predicted from the measured misfit. Treacy and Gibson (1986) observed that TEM images are affected by the bending of the layers.
X-ray rocking-curve analysis by Cembali and Servidori (1989) agreed with the elasticity calculations of curvature.

Suhir (1986) further extended Timoshenko's analysis to deal with variation of stress along the bimetallic strip by allowing for end effects associated with a finite layer. Nakajima (1992) provided an alternative derivation.

**Surfaces**

Film-edge-induced stresses were considered by Hu (1978), whose calculation was based on a concentrated point-force at the film edge. Later [Hu (1979)] the analysis was modified to allow for a force distributed over a region near the film edge. The benefit of the distributed-force model was highlighted by Fischer (1983) when he showed that the forces calculated using the concentrated point-force model were high enough to generate dislocations. In practice dislocations were not seen and the distributed-force model with its lower stresses was vindicated. Using the analysis developed for finite bimetallic strips, Luryi and Suhir (1986) proposed a method of obtaining very high critical thicknesses by allowing strained overlayers to relax. Fischer and Richter (1992) continued work on film-edges to develop a model for a finite rectangular film grown on a rigid substrate, which they extended in 1994 to allow for a 'soft' substrate.

Based on Suhir's suggested mechanism of obtaining high critical thickness, Atkinson et al. (1995) studied the energetics of introducing a misfit dislocation into a finite rectangular film. It was shown that for a finite strained layer there is not only a critical thickness, but also a critical width and critical length.

The analyses for the finite overgrowths are not based on rigorous elasticity theory, for example the stresses do not always obey the equilibrium equations. For a correct strain field one must resort to FEA similar to that used by Van Miegham et al.
Buried inclusions

The study of buried inclusions can be traced to work on thermoelastic stress. If a small region of a body is heated, it expands and creates a strain field in the body. Much of this work uses the idea of point forces or 'nuclei of strain'. Mindlin and Cheng (1950) give a good example of their use when they solve the problem of a spherical inclusion near a free surface. They observed a large increase, a factor of $4(1 + \nu)$, in the stress near a free surface compared to that in an infinite medium.

Eshelby (1957) used the idea of a point force to derive a formula for the strain field of an ellipsoidal inclusion in an infinite medium, which formed the basis of the work on quantum-wire arrays by Gosling and Willis (1995).

The cuboidal inclusion near a surface has been solved numerically by Chiu (1978). Glas (1991) solved the same problem analytically through Fourier expansion by using the solution for an elementary sinusoidal dilatation of a layer near a surface.

The effect of anisotropy on the strain in buried wires has been treated by De Caro and Tapfer (1994), although they ignored relaxation. The buried layer has been treated through FEA by Faux et al. (1994).

2.1.4 Fourier-series method

Of the two computational methods for calculating strain fields, FEA is not applicable to the geometry of many strained-layer structures and BEA requires considerable work to implement. The analytic solutions available are often very complicated, may be incorrect, or require numerical solutions to differential equations.

In this scenario, a simple analytic method for calculating the strain fields of strained-layer structures is desirable. Analytic functions are more useful if the calculated strain fields are to be used as the basis for further analysis of, for example, critical thickness or electronic properties. None of the techniques described above provide the required simple analytic method.
Faux has developed a technique based on expressing surface stresses as Fourier series which can be used to calculate the strain field of an arbitrary normal stress distribution applied to a rectangular block [Faux and Haigh (1990), Faux (1994), Faux and Gill (1994)]. Faux' analysis is an extension of the work by Pickett (1944) and, to a lesser extent, of Timoshenko (1970). The Fourier-series method, as Faux' work will now be referred, does not give a simple analytic solution; but it is almost as useful because it can calculate the strain field at any point within the rectangular block to any desired degree of accuracy. The work in this chapter will extend Faux' analysis and will suggest how several blocks can be linked together to allow strain calculations on more complicated geometries.

2.2 The single block

Figure 2.1 shows the problem tackled in this section.

![Figure 2.1: An elastic block subjected to normal and tangential tractions on all four sides.](image)

A solution to the problem for arbitrary stresses applied on the four surfaces is required. It will be assumed that the boundary conditions can be expressed as Fourier series. The assumption limits the method to functions that are piecewise continuous on the boundary, but is not a drawback for most physical situations.

Having assumed Fourier-like boundary conditions, it is useful to take a stress function
of the form:

\[
\phi(x, y) = \frac{1}{2}\sigma_{xx}x^2 + \frac{1}{2}\sigma_{yy}y^2 - \sigma_{xy}xy \\
+ \sum_{i=1}^{\infty} A_i^\pm \cos \alpha_i x \ h_i^\pm(y) + B_i^\pm \sin \alpha_i x \ h_i'^\pm(y) \\
- \sum_{i=1}^{\infty} C_i^\pm \sin \alpha_i x \ i_i^\pm(y) - D_i^\pm \cos \alpha_i x \ i_i'^\pm(y) \\
+ \sum_{i=1}^{\infty} E_i^\pm \cos \beta_i x \ j_i^\pm(x) + F_i^\pm \sin \beta_i x \ j_i'^\pm(x) \\
- \sum_{i=1}^{\infty} G_i^\pm \sin \beta_i x \ k_i^\pm(x) - H_i^\pm \cos \beta_i x \ k_i'^\pm(x),
\]

(2.1)

where \(\alpha_i, \alpha'_i, \beta_i\) and \(\beta'_i\) are Fourier frequencies, for example \(\frac{\pi}{4}\) or \(\frac{(\pi-1)\pi}{8}\). \(A_i, B_i, C_i, D_i, E_i, F_i, G_i\) and \(H_i\) are constants which will be referred to as the Fourier coefficients of the stress function. The functions \(h_i(y), i_i(y), j_i(x), k_i(x), h'_i(y), \text{etc.}\) will be referred to as fitting functions. The functions \(h_i^+(y)\) and \(h_i'^+(y)\) are different functions, each being associated with either the cosine or sine terms of the Fourier expansion respectively. The dash superscripts appearing before the ‘\(\pm\)’ do not indicate differentiation; therefore, differentiation will only be denoted by dash superscripts appearing after the ‘\(\pm\)’ superscripts. The superscript ‘\(\pm\)’ indicates that each line represents two sums, one where the constants and functions have positive superscripts and one where they have negative superscripts. These refer to terms which can be associated with the upper and lower, or left and right, surfaces respectively.

It is clear that this stress function will result in expressions for the stresses which will be of a very similar form to the boundary conditions. The exact choice of the Fourier frequencies and the fitting functions will determine the detail of the mathematics, but in all cases it is the Fourier coefficients of the stress function that will be sought. For most problems the coefficients of the stress function and the boundary conditions will have similar values. The analysis for the general case will be presented first, and later the consequences of choosing particular frequencies and fitting functions will be discussed.

The stress-function must be a solution of equation 1.12 which means that,

\[
h_i^\pm(y) = h_{C1i}^\pm \cosh \alpha_i y + h_{C2i}^\pm \sinh \alpha_i y + h_{C3i}^\pm y \cosh \alpha_i y + h_{C4i}^\pm y \sinh \alpha_i y,
\]

(2.2)
where $h_{11}^\pm$, $h_{21}^\pm$, $h_{31}^\pm$, $h_{41}^\pm$ are arbitrary constants; similar expressions for $i_1^\pm(y)$, $j_1^\pm(y)$ and $k_1^\pm(y)$, and the ‘dashed’ functions can be found. The four arbitrary constants of the eight sets of fitting functions can be chosen in any manner, but later it will be shown that certain choices greatly simplify the mathematics.

To solve the general problem illustrated in figure 2.1, a set of stress-function coefficients is required that will satisfy the boundary conditions. To this end, the stresses derived from the stress function must be equal to the applied boundary stresses at the appropriate boundary. The stresses are easily obtained from the stress function by differentiating twice, according to equations 1.11. For example, $\sigma_{xx}(x, y)$ is given by

$$\sigma_{xx}(x, y) = \sigma_{xx} + \sum_{i=1}^{\infty} A_i^\pm \cos \alpha_i x \ h_i^{\pm\prime\prime}(y) + B_i^\pm \sin \alpha_i x \ h_i^{\pm\prime\prime}(y)$$

$$- \sum_{i=1}^{\infty} C_i^\pm \sin \alpha_i x \ i_i^{\prime\prime}(y) - D_i^\pm \cos \alpha_i x \ i_i^{\prime\prime\prime}(y)$$

$$- \sum_{i=1}^{\infty} F_i^\pm \beta_i^2 \cos \beta_i y \ j_i^\pm(x) + F_i^\pm \beta_i^2 \sin \beta_i y \ j_i^\pm(x)$$

$$+ \sum_{i=1}^{\infty} G_i^\pm \beta_i^2 \sin \beta_i y \ k_i^\pm(x) - H_i^\pm \beta_i^2 \cos \beta_i y \ k_i^\pm(x), \quad (2.3)$$

and by setting $x = +1$ the normal stress at the right-hand surface of the elastic block is obtained:

$$\sigma_{xx}(1, y) = \sigma_{xx} + \sum_{i=1}^{\infty} A_i^\pm \cos \alpha_i 1 \ h_i^{\pm\prime\prime}(y) + B_i^\pm \sin \alpha_i 1 \ h_i^{\pm\prime\prime}(y)$$

$$- \sum_{i=1}^{\infty} C_i^\pm \sin \alpha_i 1 \ i_i^{\prime\prime}(y) - D_i^\pm \cos \alpha_i 1 \ i_i^{\prime\prime\prime}(y)$$

$$- \sum_{i=1}^{\infty} F_i^\pm \beta_i^2 \cos \beta_i y \ j_i^\pm(1) + F_i^\pm \beta_i^2 \sin \beta_i y \ j_i^\pm(1)$$

$$+ \sum_{i=1}^{\infty} G_i^\pm \beta_i^2 \sin \beta_i y \ k_i^\pm(1) - H_i^\pm \beta_i^2 \cos \beta_i y \ k_i^\pm(1). \quad (2.4)$$

This stress can be set equal to the boundary stress, which gives an equation relating all of the unknown Fourier-coefficients of the stress-function to the known Fourier coefficients of the normal stress imposed on the right-hand surface. Suppose the boundary condition for the normal stress on the right-hand surface is

$$\sigma_{xx}(l, y) = \sigma_{xx} + \sum_{i=1}^{\infty} W_i^+ \cos \beta_i y + X_i^+ \sin \beta_i y. \quad (2.5)$$
On multiplying equations 2.4 and 2.5 by \( \cos \beta y \) and integrating with respect to \( y \) from \(-c\) to \(+c\), it is possible to equate terms of equal frequency. In other words, before equating terms of equal frequency, the fitting functions are expanded as Fourier series. The following relationship holds for the \( W_r^+ \),

\[
W_r^+ = \sum_{i=1}^{\infty} \alpha_i \int_{-c}^{c} h_i^{\pm}(y) \cos \beta_r y \, dy + B_i^+ \int_{-c}^{c} h_i^{\pm}(y) \sin \alpha_i y \, dy
\]

\[
+ \sum_{i=1}^{\infty} C_i^\pm \cos \alpha_i \int_{-c}^{c} i_i^\pm(y) \cos \beta_r y \, dy + D_i^\pm \sin \alpha_i \int_{-c}^{c} i_i^\pm(y) \sin \beta_r y \, dy
\]

\[
- \{ E_r^\pm \beta_r^2 \beta^2 \kappa_r(l) + G_r^\pm \beta_r^2 \kappa_r(l) \} c \quad \forall r,
\]

(2.6)

where \( i \) and \( r \) are integers, \( W_r^+ \) is the \( r \)th cosine Fourier coefficient of the normal stress on \( x = +l \) and \( A_i^\pm, B_i^\pm, C_i^\pm, D_i^\pm, E_r^\pm \) and \( G_r^\pm \) are Fourier coefficients of the stress function.

It is possible to derive a total of sixteen sets of equations of this type, involving each of the sixteen Fourier coefficients of the boundary conditions, \( A_i^\pm, B_i^\pm, C_i^\pm, D_i^\pm, E_r^\pm \) and \( G_r^\pm \) are Fourier coefficients of the stress function. Suitable choice of the Fourier frequencies and the fitting functions can greatly simplify the solving of equations 2.6.

The Fourier frequencies must be chosen such that the trigonometric functions form a basis set, which allows at least the combinations shown in Table 2.1. The analysis from this point onwards depends on the choice of the Fourier frequencies.

<table>
<thead>
<tr>
<th></th>
<th>( \alpha_i )</th>
<th>( \beta_i )</th>
<th>( \alpha_i^\prime )</th>
<th>( \beta_i^\prime )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>( \frac{ix}{l} )</td>
<td>( \frac{ix}{c} )</td>
<td>( \frac{ix}{l} )</td>
<td>( \frac{ix}{c} )</td>
</tr>
<tr>
<td>(2)</td>
<td>( \frac{ix}{l} )</td>
<td>( \frac{ix}{c} )</td>
<td>( \frac{(i-\frac{1}{2})x}{l} )</td>
<td>( \frac{(i-\frac{1}{2})x}{c} )</td>
</tr>
<tr>
<td>(3)</td>
<td>( \frac{(i-\frac{1}{2})x}{l} )</td>
<td>( \frac{(i-\frac{1}{2})x}{c} )</td>
<td>( \frac{ix}{l} )</td>
<td>( \frac{ix}{c} )</td>
</tr>
</tbody>
</table>

Table 2.1: Fourier frequencies that form basis sets.
2.3 Normal and shear tractions

The shear stress is obtained from the stress function by differentiating once with respect to \( x \) and once with respect to \( y \):

\[
\sigma_{xy}(x, y) = \sigma_{XY} + \sum_{i=1}^{\infty} \alpha_i A_i^\pm \sin \alpha_i x \ h_i^\pm(y) - \alpha_i' B_i^\pm \cos \alpha_i' x \ h_i'^\pm(y)
\]

\[
- \sum_{i=1}^{\infty} \alpha_i C_i^\pm \sin \alpha_i x \ i_i^\pm(y) + \alpha_i D_i^\pm \cos \alpha_i x \ i_i'^\pm(y)
\]

\[
+ \sum_{i=1}^{\infty} \beta_i E_i^\pm \sin \beta_i y \ j_i^\pm(x) - \beta_i' F_i^\pm \cos \beta_i' y \ j_i'^\pm(x)
\]

\[
- \sum_{i=1}^{\infty} \beta_i G_i^\pm \sin \beta_i y \ k_i^\pm(x) + \beta_i' H_i^\pm \cos \beta_i' y \ k_i'^\pm(x).
\] (2.7)

Therefore, by choosing the second set of frequencies it is possible to obtain very simple expressions for the shear stresses at the boundaries. If this is combined with a choice of fitting functions such that the first derivatives of all, except one, are equal to zero at the boundary;

\[
i_i^\pm(+l) = k_i^{-\prime}(+l) = 0, \quad k_i^{+\prime}(+l) = -\frac{1}{\beta_i},
\]

\[
i_i^{\prime\prime\prime}(+l) = k_i^{^{-\prime\prime\prime}}(+l) = 0 \quad \text{and} \quad k_i^{+\prime\prime\prime}(+l) = -\frac{1}{\beta_i};
\]

then the shears at the boundaries have the following form,

\[
\sigma_{xy}(+l, y) = \sigma_{XY} + \sum_{i=1}^{\infty} G_i^\pm \cos \beta_i y + H_i^\pm \sin \beta_i' y.
\] (2.8)

Clearly the coefficients of the stress function, \( G_i^\pm, D_i^\pm, G_i^\pm \) and \( H_i^\pm \) are equal simply to the corresponding coefficients of the boundary conditions.

Equation 2.6 for the normal stresses can similarly benefit from suitable choice of frequencies and fitting functions. Keeping to the frequencies chosen above and setting \( j_i^+(l) = -\frac{1}{\beta_i}, j_i^-(l) = 0 \) and \( k_i^\pm(l) = 0 \) equation 2.6 reduces to

\[
W^+ c = E^+_c c + \sum_{i=0}^{\infty} (-1)^i \left\{ A_i^\pm \int_{-c}^{+c} h_i^{\pm\prime\prime\prime}(y) \cos \beta_i y dy - B_i^\pm \int_{-c}^{+c} h_i^{\prime\prime\prime\prime\prime}(y) \cos \beta_i y dy \right\}.
\] (2.9)

Given a reasonable guess at the correct solution, sets of equations similar to 2.9 can often be solved by iterative methods. There are sixteen sets of Fourier coefficients, which
are found by using equation 2.9 and others similar to it, to calculate sixteen new sets of coefficients, treating each set in turn. One calculation of all sixteen sets of coefficients is known as a single iteration.

All the coefficients might change in each iteration, but the fitting functions remain unchanged. The expression for $\sigma_{xx}(\pm l, y)$ obtained from the stress function (equation 2.3) can be split into a Fourier-series like part (summation involving the E, F, G, H coefficients) and a function of $y$ (summation involving the A, B, C, D coefficients). The function of $y$ represents the influence of the top and bottom boundary conditions at the left and right sides. The iteration procedure finds a set of E, F, G, H such that the fourier-series part of equation 2.3, added to the function of $y$, is equal to the boundary condition.

By choosing the second set of Fourier frequencies, the equations based on the shear stresses at the boundaries are simplified to the extent that, the fourier coefficients, $C_r^\pm$, $D_r^\pm$, $G_r^\pm$ and $H_r^\pm$, do not change during the iterations. If a suitable initial choice is made for the coefficients, then, after a number of iterations, the coefficients will converge to the correct solution, with a closer convergence for a larger the number of iterations.

It seems apparent that a sensible starting choice for the iterative procedure is to set the coefficients of the stress function equal to the coefficients of the boundary conditions. For the simple relationships obtained by using the second set of Fourier frequencies, it is absolutely necessary to have the coefficients, $C_r^\pm$, $D_r^\pm$, $G_r^\pm$ and $H_r^\pm$, set equal to the boundary Fourier-coefficients because they do not change during the iterative procedure and, as equation 2.8 implies, they should be equal to the boundary Fourier-coefficients. This means for example, setting

$$E_i^+ = W_i^+, \quad E_i^- = W_i^-, \quad F_i^+ = X_i^+, \ldots$$ (2.10)

In this way an approximate solution of the system of equations can be obtained, the accuracy of which will depend on the number of terms in the series. When the Fourier coefficients have been found it is simple to calculate the stresses and subsequently strains and displacements for a problem. The stresses can be calculated using equations 2.3, 2.7 and a similar equation for $\sigma_{yy}(x, y)$; and, from the stresses, the strains are found using Hooke’s law. The displacements are obtained by integrating the strains, which is discussed
in more detail in section 2.4.1

The iteration procedure is carried out using a computer. Figure 2.2 is a flow chart illustrating the structure of the program. The Fourier coefficients of the boundary conditions are calculated and written to the file ‘bndcdns.dat’. This file is used as input to the main iteration routine and also to check the boundary conditions by reconstructing the function with the ‘recon’ routine. The ‘main’ routine first sets up all the functions which do not vary through the calculation (principally those functions involving the fitting functions) and then performs the iteration in the ‘iteratn’ routine. Each of the routines ‘_sur_s’ carries out the iteration associated with one set of equations 2.8 or 2.9 and ‘err_chk’ tests for convergence. Usually convergence is taken to have occurred when the difference between the current and previous values for all of the coefficients is less than 1%. The converged coefficients are output to ‘coeffs’. The stresses and strains are calculated using equations 2.3 and Hooke’s laws. The ‘.edg’ files contain 2-D plots of the stress along the surface which can be used to check that the boundary conditions are satisfied. Contour plots of the stress and strain fields appear in ‘.cnt’ files. The ‘.bnd’ and ‘.edg’ files are in a format suitable for ‘xvgr’\(^2\) and the ‘.cnt’ files for use with ‘contour’\(^3\).

The time consuming parts of the procedure are the iteration and the calculation of stresses from the coefficients. For a run using 400 terms, the whole process takes approximately 4 hours on a Sun SPARCstation \(^4\). More importantly, when compared to FEA which requires large amounts of memory, for 400 terms the program requires less than 2 megabytes of memory.

Figure 2.3 shows plots of the reconstructed boundary conditions and the stress at the surface calculated using the Fourier-series program, for a top-hat normal stress. The plots are shown with increasing numbers of terms in the stress function. The poor convergence of fourier series when used to express discontinuous functions is shown by the lack of definition at the corners of the top hat.

\(^2\)Xvgr Version 2.10 (1993) ©by P. J. Turner
\(^3\)Contour Version 3.0 (1991) written by K. K. H. Toh
\(^4\)Sun Microsystems Inc., 2550 Garcia Avenue, Mountain View, California 94043-1100, U. S. A.
Figure 2.2: A flow diagram illustrating the structure of the fourier series program. Routines are shown in normal font and input and output files are shown in italics.
Figure 2.3: The boundary force in arbitrary units (solid line) is shown, together with the calculated stress at the surface (open circles), for a top-hat function of width 20 units centred at the centre of the surface. Several plots with increasing numbers of Fourier terms are displayed. The inserts show the stress at the edge of the block (left insert) and the stress at the centre (right insert). The dimensions used, for the block shown in figure 2.1, are $l = 100$ and $c = 100$. 
The discrepancy between the boundary conditions and the calculated stress at the edge of the block is an artefact of the Fourier-series method and not a numerical error. Figure 2.4

![Figure 2.4](image)

Figure 2.4: The boundary stress calculated using 20 terms, split into the Fourier series part (dotted line) and the function of \( y \) (solid line). Figure 2.3 shows the two parts summed.

shows the stress, calculated using 20 terms, split into the Fourier-series part and the function of \( y \), previously mentioned on page 27. The Fourier-series part is equal to the boundary condition less the function of \( y \). However, the function of \( y \) is symmetrical with a discontinuity of derivative at \( x = \pm l \). A function of this form cannot be represented perfectly by a Fourier series because all the trigonometric functions have continuous derivatives at \( x = \pm l \), and, therefore, an error will occur at the edge of the block. The degree to which this error extends into the block is reduced by increasing the number of Fourier terms used, but at the point \( x = \pm l \) there will always be an error. Figure 2.5 is a plot of \('x^2'\) and the reconstructed Fourier expansion. It shows clearly the way in which the expansion has a continuous derivative through the boundary compared to the discontinuity of the function itself.

**The earlier Fourier-series method**

The analysis of Faux (1994) follows the approach described in this section, but does not include the terms in the stress function that give shears on the surface, therefore his solution is limited to normal tractions on the surface. If the terms in the stress function which give rise to the shear stresses are not included, then equation 2.9 is still correct and needs no
2.4 The prospects for linked-block strain calculations

A finite strained over-layer, shown in figure 2.6, can be modelled as four distinct, but linked, elastic blocks with appropriate boundary and interface conditions. In a similar fashion, a buried layer may be modelled by several linked blocks which are shown in figure 2.7

At any surface through a continuous elastic medium there is continuity of normal and
Figure 2.7: A buried layer can be modelled using several elastic blocks linked by appropriate interface conditions. The surface ABCDLHONMLIE is stress free, there is continuity of stress and displacement across BF, CG, GH, KL, KN, JM, JI, and FE, but across FGKJ the stress is continuous and the displacement is not.

tangential stresses, normal and tangential strains, and displacements. For a discontinuous elastic medium, a strained layer for example, there may be a discontinuity of strain and displacement across the interfaces, but the normal and tangential stresses are continuous across all interfaces in the material.

Therefore, the process of linking two rectangular blocks together, forming effectively one continuous block, requires that the normal and tangential stresses, strains and displacements of the two blocks are equal at the surfaces to be joined. Once two blocks have been linked, further blocks can be added to create more complicated shapes, and ultimately, by allowing for discontinuity of displacements, the analysis can be extended to link blocks in a 'discontinuous manner'.

2.4.1 Displacements as boundary conditions

The first step in the linking of the blocks is to develop a method of calculating the strain state of a block with either stresses or displacements imposed as boundary conditions. One would expect that an extension of the analysis of sections 2.2 and 2.3 would be adequate. This would involve finding an expression for the displacements at the boundary (similar to equation 2.3 for stress), equating it to some boundary condition and thus deriving an equation similar to 2.6.

The choice of Fourier frequencies in sections 2.2 and 2.3 simplified the analysis, par-
particularly regarding the shear stresses. However, by choosing \( \alpha_i' = \frac{(i-\frac{1}{2})\pi}{l} \), the expressions for the tangential stresses are reduced so that the tangential-stress expression evaluated at one surface is not affected by the boundary conditions of any of the other surfaces; only the normal-stress expressions are affected by the conditions at the other surfaces. This situation is ideal if all the boundary conditions can be specified, but when linking blocks that is not possible.

At the surface common to both blocks, the stresses are unknown; therefore, a boundary condition cannot be imposed, and equation 2.6 is of no use. Instead, expressions for the tangential stresses at the interface which involve terms arising from the stresses applied to the other surfaces are required. Normal and shear stresses at the interface, appropriate to the stresses applied to the surfaces, can then be calculated.

To obtain such expressions for the stress it is necessary to choose standard Fourier frequencies (the first set in table 2.1); if either of the other two sets are chosen, then one of the expressions for stress is simplified to the extent that it is independent of all except two Fourier coefficients, resulting in equations similar to 2.8. So, when standard Fourier-frequencies are used, the normal and tangential stresses at \( x = +l \) are given by

\[
\sigma_{xx}(+l, y) = \sigma_{xx} + \sum_{i=1}^{\infty} A_i^{\pm}(-1)^i h^{\pm''}_i(y) + \sum_{i=0}^{\infty} D_i^{\pm}(-1)^i h^{\pm''}_i(y) \\
- \sum_{i=0}^{\infty} \beta_i^2 (E_i^{\pm} \cos \beta_i y + F_i^{\pm} \sin \beta_i y) j_i^{\pm}(+l) \\
+ \sum_{i=0}^{\infty} \beta_i^2 (G_i^{\pm} \sin \beta_i y + H_i^{\pm} \cos \beta_i y) k_i^{\pm}(+l)
\]

and

\[
\sigma_{xy}(+l, y) = \sigma_{xy} - \sum_{i=1}^{\infty} \alpha_i B_i^{\pm}(-1)^i h^{\pm'}_i(y) + \sum_{i=0}^{\infty} \alpha_i C_i^{\pm}(-1)^i h^{\pm'}_i(y) \\
+ \sum_{i=0}^{\infty} \beta_i (E_i^{\pm} \sin \beta_i y - F_i^{\pm} \cos \beta_i y) j_i^{\pm'}(+l) \\
+ \sum_{i=0}^{\infty} \beta_i (G_i^{\pm} \cos \beta_i y + H_i^{\pm} \sin \beta_i y) k_i^{\pm'}(+l),
\]

which, when equated to the boundary conditions, multiplied by \( \cos \beta_r l \) and integrated with respect to \( y \) from \(-c\) to \(+c\), give the following equations:

\[
cE_r^+ = cW_r^+ - \sum_{i=0}^{\infty} A_i^{\pm}(-1)^i \int_{-c}^{+c} h^{\pm''}_i(y) \cos \beta_r y dy
\]
\[ + \sum_{i=0}^{\infty} D_i^\pm (-1)^i \int_{-c}^{+c} t_i^{\pm'}(y) \cos \beta_i y dy \]

and

\[ \alpha_i B_i^\pm (-1)^i \int_{-c}^{+c} h_i^{\pm'}(y) \cos \beta_i y dy \]

\[ + \sum_{i=0}^{\infty} \alpha_i C_i^\pm (-1)^i \int_{-c}^{+c} t_i^{\pm'}(y) \cos \beta_i y dy. \]  

(2.13)

The strains are obtained from the displacements by differentiation:

\[ \epsilon_{xx} = \frac{\partial u}{\partial x}, \quad \epsilon_{xy} = \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \quad \text{and} \quad \epsilon_{yy} = \frac{\partial v}{\partial y}, \]  

(2.15)

thus the displacements can be obtained by integrating the strains.

Figure 2.8: Two simple paths, of the many possible, along which strains can be integrated to find the displacement.

If the centre of a block is taken to have zero displacement, then by following one of the two paths shown in Figure 2.8 the displacements are: from path A,

\[ u(+l, y) = \int_0^{+l} \epsilon_{xx}(x', 0) dx' + \int_0^{+l} \epsilon_{xy}(+l, y') dy' \]

\[ v(+l, y) = \int_0^{+l} \epsilon_{xy}(x', 0) dx' + \int_0^{+l} \epsilon_{yy}(+l, y') dy', \]

or from path B,

\[ u(+l, y) = \int_0^{+l} \epsilon_{xy}(0, y') dy' + \int_0^{+l} \epsilon_{xx}(x', y) dx' \]

\[ v(+l, y) = \int_0^{+l} \epsilon_{yy}(0, y') dy' + \int_0^{+l} \epsilon_{xy}(x', y) dx'. \]

The integration of the expressions from path A is easier and produces simpler results, and is therefore used to find the displacements. Nevertheless, the displacements derived in this way are very complex because a large number of terms is involved. For example,
\[ u(l, y) \text{ is} \]

\[
\frac{1 + \nu}{E} \left\{ \begin{array}{l}
\sum_{i=1}^{\infty} \frac{B_i^+}{\alpha_i^+} \left[ (1 - \nu) h_i^{++}(0) + \alpha_i^2 \nu h_i^{++}(0) \right] \\
+ \sum_{i=1}^{\infty} \frac{D_i^+}{\alpha_i^+} \left[ (1 - \nu) a_i^{++}(0) + \alpha_i^2 \nu a_i^{++}(0) \right] \\
- \sum_{i=0}^{\infty} E_i^+ \left[ \beta_i^2 \left(1 - \nu\right) \int_0^1 j_i^+(x) dx + \nu \int_0^1 j_i^{++}(x) dx \right] \\
- \sum_{i=0}^{\infty} G_i^+ \left[ \beta_i^2 \left(1 - \nu\right) \int_0^1 k_i^+(x) dx + \nu \int_0^1 k_i^{++}(x) dx \right] \\
+ \frac{1 + \nu}{E} \sum_{i=0}^{\infty} \frac{G_i^+}{\beta_i} \left(1 - \cos \beta_i y\right) - \frac{H_i^+}{\beta_i} \sin \beta_i y
\end{array} \right\} (2.16)
\]

These displacements can be used in the same way as equations 2.3 in section 2.3 to generate a set of iteration equations relating each coefficient of the stress function to the other coefficients, and subsequently the block with stresses or displacements as boundary conditions can be solved.

The Fourier-series-like stress function is chosen to provide simple expressions for the stresses and, as seen above, it gives complicated expressions for displacements. Although it is simple to express the displacement boundary conditions as Fourier series, it is not clear what a suitable starting guess for the iteration procedure will be; certainly the coefficients of the stress function will not be similar to the coefficients of the displacement boundary-conditions.

An initial guess of zero for the stress-function coefficients that are associated with the displacement boundary conditions does not give convergence. This contrasts with the coefficients associated with the stresses, which take only a few iterations more than the usual figure of approximately ten iterations when the initial guess is set to zero rather than to the boundary conditions.

It will be possible to derive suitable initial guesses for the displacement coefficients by equating the stress-function displacements to the boundary condition displacements, and ignoring all the terms from the stress function that are not directly concerned with that displacement.
2.4.2 Linked blocks

In order to link blocks and thus perform strain calculations for a wider range of structures, it is first necessary to develop a computer program based on equation 2.16 and others similar to it, which enables displacements to be specified on the boundaries of a single block. Once this has been achieved separate blocks may be linked.

The iteration equations for the stress-function coefficients at the surfaces of the blocks will be the same as those used earlier, but for the coefficients at the interface between two blocks the iteration equations need to be modified. Instead of setting the stress at the interface equal to a boundary condition, it must equal the stress at the interface calculated from the stress function of the adjacent block. For example, for the two blocks shown in

\[
\begin{align*}
\sigma_{xx} &= \sigma_{xx} \\
\sigma_{xy} &= \sigma_{xy}
\end{align*}
\]

Figure 2.9: By using appropriate boundary conditions, two elastic blocks can be linked to form a single continuous elastic block.

Figure 2.9, the stresses and displacements at the right side of block A (or block \(n,m\)) must be equal to those at the left side of block B (or block \(n,m + 1\)). Therefore, from the continuity of the normal stress across the interface, the iteration equation will be

\[
\begin{align*}
\sum_{i=1}^{\infty} A_i^{n,m} \cos \alpha_i l \int_{-c}^{+c} h_i^{n,m}''(y) \cos \beta_r dy + B_i^{n,m} \sin \alpha_i l \int_{-c}^{+c} h_i^{n,m}''(y) \cos \beta_r dy \\
+ \sum_{i=1}^{\infty} C_i^{n,m} \cos \alpha_i l \int_{-c}^{+c} i_i^{n,m}''(y) \cos \beta_r dy + D_i^{n,m} \sin \alpha_i l \int_{-c}^{+c} i_i^{n,m}''(y) \cos \beta_r dy \\
- \left\{ E_i^{n,m} \beta_r^2 j_i^{n,m}(+l) + G_i^{n,m} \beta_r^2 k_i^{n,m}(+l) \right\} c = 0
\end{align*}
\]
\[
\sum_{i=1}^{\infty} A_i^{n,m+1\pm} \cos \alpha_i \int_{-c}^{+c} h_i^{n,m+1\pm}(y) \cos \beta_i \, dy + B_i^{n,m+1\pm} \sin \alpha_i \int_{-c}^{+c} h_i^{n,m+1\pm}(y) \cos \beta_i \, dy \\
+ \sum_{i=1}^{\infty} C_i^{n,m+1\pm} \cos \alpha_i \int_{-c}^{+c} t_i^{n,m+1\pm}(y) \cos \beta_i \, dy + D_i^{n,m+1\pm} \sin \alpha_i \int_{-c}^{+c} t_i^{n,m+1\pm}(y) \cos \beta_i \, dy \\
- \left\{ E_r^{n,m+1\pm} \beta_r^2 j_{r,n,m+1\pm}^{r,-1}(-l) + G_r^{n,m+1\pm} \beta_r^2 k_{r,n,m+1\pm}^{r,-1}(-l) \right\} c \quad \forall \tau, \quad (2.17)
\]

where the additional superscripts on the Fourier-coefficients and the fitting-functions label the block to which they apply.

The tangential stress and the normal and tangential displacements will give equations similar to equation 2.17. The same equations will be used to calculate the coefficients of the blocks on both sides of the interface: instead of two sets of equations for two sets of coefficients, there will be four sets of equations for four sets of coefficients.

The mathematical complexity of equation 2.17 means that a program using it is difficult to write and, to some extent, the elegant simplicity of the Fourier-series method for the single block is lost. A fully working, linked-block, Fourier-series method program would be advantageous for some problems. However, some structures, such as buried strained-layers or quantum-wire lasers, can be better treated using other methods. One such method is presented in chapter 4.
Chapter 3

Applications of the Fourier-Series Method

The theory described in the previous chapter is used to analyse three problems: a TEM 90°-wedge sample, strain relaxation at the facets of quantum-well lasers, and a buried layer near a free surface. The details and results of these calculations are presented in sections 3.1, 3.2 and 3.3. A Fourier-integral method, based on the Fourier-series method, is presented in section 3.4.

3.1 TEM 90°-wedge sample

Transmission electron microscopy (TEM) involves firing an electron beam at a suitably thin sample and observing the subsequent diffraction patterns. By using a lens to refocus the beam, a contrast pattern is obtained which can be used to determine the lattice spacing in a sample. Consequently, a strained sample produces a different TEM contrast pattern to an unstrained sample, and this effect can be used to measure the strain in strained-layer structures. However, the strain relaxes at the surfaces of the thin samples and this affects the contrast patterns. The relaxation needs to be accounted for if TEM is to measure the unrelaxed strain of layers.
Harvey et al. (1992) and Faux and Gill (1994) have examined this problem in detail, in order to develop such a strain-measuring technique. The sample they considered was a 90°-wedge sample with the normal to the plane of the strain layer running parallel to both surfaces, shown in figure 3.1(a). Calculating the relaxation of a sample with this geometry requires dealing only with stresses normal to the surfaces; however, it does require a three-dimensional analysis. Harvey et al. (1992) used FEA to calculate the strains and, later, Faux and Gill (1994) developed a three-dimensional Fourier method.

Samples with other geometries are studied using TEM. A sample in which the normal to the plane of the strained layer is at 45° to both surfaces of the sample has been considered by Chou et al. (1994). If the wedge is thick enough, then the strain relaxation for this sample, shown in figure 3.1(b), can be calculated assuming plane strain conditions.

In order to model the free surfaces of the sample, it is necessary to cancel the in-plane stress of the layer at the surfaces. This can be achieved by subtracting the stress distribution of an elastic block under traction equal in magnitude to the in-plane stress, applied on each surface. The stress field used to cancel the in-plane stress at the surface is known as the relaxation stress-field.

For the 90°-wedge sample in figure 3.1 (b) the in-plane stress is not perpendicular to the surfaces, and, therefore, has a tangential component at the surface. The stresses required to cancel the in-plane stress at the surface are shown in figure 3.2. The tangential component means that the analysis of Faux and Gill (1994) could not be used to calculate the strain field, although of course FEA could be used.

The Fourier-series method described in sections 2.2 and 2.3 has been used to calculate
Figure 3.2: Geometry of the TEM sample used in the strain calculation showing the boundary stresses used to calculate the strain relaxation.

the strain field of the structure in figure 3.2. The calculations were performed using 500 Fourier terms and, in order to calculate the strains, the elastic constants for GaAs were taken from Fitzgerald (1993) and are $E = 8.5 \times 10^{10} \text{Nm}^{-2}$ and $\nu = 0.312$. The results are shown in figure 3.3 as contour plots.

The important features are the top-hat functions for the tangential and normal stresses at the appropriate corners in figures (c), (d) and (e), and the symmetrical shape of figures (b) and (f) for the in-plane strain, $\frac{1}{\sqrt{2}}(\epsilon_{xx} + \epsilon_{yy})$, and the in-plane stress, $\frac{1}{\sqrt{2}}(\sigma_{xx} + \sigma_{yy})$. The amount of relaxation of the in-plane strain is large at points A and B in figure 3.2, which one would expect because the layer is constrained by less material on the AB side. The relaxation of the in-plane strain along the centre of the layer is plotted as a function of distance in figure 3.4; it compares favourably to the $\frac{1}{r}$ dependence observed by Faux (1994) for a strained layer at right angles to the surface. However, the geometry of Faux' layers meant that the two relaxing surfaces were effectively isolated, whereas, for the TEM sample studied here, the stresses of the two surfaces interact; together with the different geometry, this means one would not expect an exact $\frac{1}{r}$ dependence.
Figure 3.3: Contour plots of the stresses and strains of the TEM sample shown in figure 3.1. The absolute strain contours are labelled in units of $10^{-3}$ and the stresses are labelled in units of $10^7$ Nm$^{-2}$. 
3.2 Facets of strained quantum-well lasers

Strain relaxation at the end facets of strained quantum-well lasers has been recognised for some time [Faux and Haigh (1990)]. For a compressively-strained quantum-well the relaxation causes a decrease in band gap at the facet. The decrease in band gap can cause electron-hole pairs to drift to the facet, which can in turn lead to increased absorption. A high absorption near the facet is highly undesirable and could be the cause of catastrophic optical damage.

The calculation of strain relaxation has been carried out for a single uncompensated well and a strain-compensated well. The results have been used by A. Meney to calculate the optical absorption-coefficient for the well as a function of distance from the facet.

The structure of the laser is shown in figure 3.5. The cladding is grown lattice matched at the growth temperature, but because of differences in the thermal expansivity the cladding is strained by 0.1% at room temperatures.

The details of the quantum well and barrier geometries are shown in figures 3.6 and 3.7 for the strain-compensated and single strained quantum-well layers respectively. The simple strained layer is 80Å wide and is compressively-strained to 1%; whereas the strain-

\[ A. \text{ Meney, Department of Physics, University of Surrey, Guildford, Surrey, GU2 5XH.} \]
compensated layer has two additional barriers on either side, which are tensilely-strained to 1%. It should be noted that in this section the compressive strains are considered positive in accordance with the convention used by band structure theorists.

The cladding is only slightly strained to 0.1% and, therefore, cannot relax by more than this amount. Close to the facet the relaxation of the wells and barriers will be dominant, but, according to St. Venants principle, the strain of 0.1% will be relaxed much further into the layer because the cladding layers are much thicker than the wells and barriers.

The boundary stress required to calculate the relaxation of the very thick cladding layer and the very thin quantum wells and barriers together is very difficult to express accurately as a Fourier series because the range of frequencies required is too large. For this reason the relaxation of the cladding and then the wells and barriers are calculated separately, each
using 800 Fourier terms, and summed afterwards.

The relaxation of the strain in the quantum well is most important for calculations of the optical absorption, because it is in the well that there are recombining electron-hole pairs. The programs written by A. Meney, based on theory given in Yariv (1967), only treat variation in strain along the quantum-well, not across it, and, therefore, require strain as a one-dimensional function of distance from the facet. The average strain over the height of the quantum well was calculated from the two-dimensional data generated by the Fourier-series program and the results are shown in figures 3.8, 3.9 and 3.10.

![Figure 3.8: Strain relaxation arising from the 0.9% strain in the quantum well relative to the cladding. The well is 80Å wide.](image)

![Figure 3.9: Strain relaxation arising from the 0.9% strain in the quantum well relative to the cladding, for a strain-compensated quantum well. The well is 80Å wide and has a 1.0% tensilely-strained 40Å barrier either side.](image)

Comparing the two parts of the relaxation, it is clear that the relaxation of the cladding is important at long range, and that of the quantum-well is important over short range. The strain-compensated layer relaxes over a much shorter distance, although its maximum relaxation is similar to that of the uncompensated quantum well.

Figures 3.11 and 3.12 show the absorption calculated for the single quantum well and the strain-compensated quantum well. The absorption near the facet is reduced in the strain-compensated structure. Devices based on the structures used for these calculations have been grown and tested by Phillips\(^4\). The lasers tested showed improved properties and,

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together with these calculations, were the basis of a patent application.\footnote{Patent entitled 'Semiconductor Diode Laser and Method of Manufacturing' filed at the European Patent Office (Ref: PHN 15432 EP-P).}

### 3.3 The buried layer near a free surface

Most strained buried-layers lie close to the surface of the devices into which they are incorporated, but it is assumed that surface effects are negligible. However, it is conceivable that, for certain structures, the close proximity of the surface may influence the properties of the buried layer. In order to investigate this possible effect the stress field has been...
calculated for a structure which is considered more likely to be affected than most.

Figure 3.13: The cross section of a strained-quantum-well laser. All the InP regions have the same lattice parameter as the InGaAsP regions. The SiO₂ films may have a misfit relative to the InP, but will be ignored in the calculation presented here. The strained layers are of InGaAs and the unstrained barriers are of InGaAsP.

The structure is chosen on the basis that the influence of the surface will be greatest for buried layers with the largest net strain close to the surface. The structure, shown in figure 3.13, contains sixteen layers of width 25Å, length 4µm and compressively strained to 1%. These layers are buried only 1.5µm from the surface.

The stress field for the buried layer in an infinite medium is described in chapter 4. To obtain the stress field for the layer near a surface, the stresses at this surface within the infinite medium need to be cancelled. This can be achieved by using the Fourier series program to calculate the stress field associated with applying this force to the surface of a finite medium, and then subtracting this stress field from that of the layer buried in an infinite medium.

The stress field for sixteen buried layers in an infinite medium is obtained by superposing sixteen stress-fields for a single layer. The stress field for sixteen layers in cartesians is too large to display here, instead the field for only one layer is given, but the actual calculations use the stress field for all sixteen layers.

The stress about a rectangular buried-inclusion is derived in chapter 4, and using this derivation the normal and tangential tractions on a surface a distance b above the centre of
a layer of length \(2l\) and thickness \(2c\) are,

\[
\sigma_{yy}(x, b) = \frac{E\epsilon_0}{2\pi(1-\nu)} \left\{ \arctan \left( \frac{c-b}{l-x} \right) + \arctan \left( \frac{c-b}{l+x} \right) \right. \\
\left. + \arctan \left( \frac{c+b}{l-x} \right) + \arctan \left( \frac{c+b}{l+x} \right) \right\}
\]

and

\[
\sigma_{xy}(x, b) = \frac{E\epsilon_0}{2\pi(1-\nu)} \left\{ \ln \left| (l+x)^2 + (c-b)^2 \right| + \ln \left| (l-x)^2 + (c+b)^2 \right| \right. \\
\left. + \ln \left| (l-z)^2 + (c-b)^2 \right| + \ln \left| (l+z)^2 + (c+b)^2 \right| \right\}.
\] (3.1)

\(\sigma_{yy}(x, b)\) and \(\sigma_{xy}(x, b)\) can be expressed as Fourier series and the programs described in chapter 2 can calculate the stress field at the surfaces of the rectangular block shown in figure 3.14. The dimensions of the rectangular block are chosen so that the surfaces \(AD\), \(CD\) and \(CB\) do not interfere with the stress near the centre of \(AB\). Subtracting the stress field of the rectangular block from that of the buried layer will leave a stress-free surface along \(AB\) in the infinite medium.

\[\text{Figure 3.14: The rectangular block indicating the stresses required to leave a free surface along } AB \text{ within the infinite medium.}\]

Provided that the stress-free surface is long compared to the length of the buried layer, the stress field close to the buried layer is that of the buried layer near a free surface. Figure 3.15 shows the stress field required to leave the surface \(AB\) of figure 3.14 stress free.
Figure 3.15: Contour plot of the stress relaxation of the 16 buried layers near the surface. The left plot shows $\sigma_{yy}$ and the right $\sigma_{x\gamma}$, the shaded rectangle shows the position of the quantum-well stack.

If this is compared to the stress field for the buried layer shown in figure 4.5, one can see that the influence of the free surface on the stresses close to the buried layers is negligible. The free surface modifies the stress field near the buried layer by less than 1%. It is therefore concluded that surface effects will have little influence on the properties of devices incorporating buried layers. The strain arising from the SiO$_2$ coatings, which is ignored here, is likely to have greater influence.

3.4 Fourier-integral method

The advantage of analytic over numerical solutions was mentioned in the introduction to this chapter. For example, if further analysis is to be carried out using the strain fields, then the analysis is invariably easier if the strain fields are analytic. To extend the possibility of analytic solutions, a method of solving analytically the problem Faux and Haigh (1990) solved using Fourier-series is given in this section.

Faux and Haigh considered an infinitely-long layer, shown in figure 3.16, using the Fourier-series method, and obtained the following Fourier sum for $\sigma_{yy}$ for a top-hat normal
force, with width $2a$ and amplitude $q$, applied at the origin:

$$\sigma_{yy} = \frac{qa}{l} - 4q \sum_{m=1}^{\infty} \frac{\sin \alpha_m a \cos \alpha_m x}{\alpha_m l} \times$$

$$\left( \frac{\alpha_m y \sinh \alpha_m c \sinh \alpha_m y - \alpha_m c \cosh \alpha_m c \cosh \alpha_m y - \sinh \alpha_m c \cosh \alpha_m y}{2\alpha_m c + \sinh 2\alpha_m c} \right),$$

where $\alpha_m a = \frac{m\pi a}{l} = u_m$ and the dimensions $a$, $c$ and $l$ are given in figure 3.16. $q$ is equal to $\frac{\sigma_{0a}}{1-\nu}$ where $\varepsilon_0$ is the misfit in the layer. The theory of Faux and Haigh is strictly only valid for large $l$, so that the free surfaces at $x = \pm l$ do not affect the strain distribution in the vicinity of the strained layer. However, the equation can be simplified by taking the limit $l \to \infty$ and converting the summation to an integral. Thus, as $l \to \infty$,

$$\sum_{m=1}^{\infty} f(\alpha_m a) \to \int_0^{\infty} f(u_m)dm = \int_0^{\infty} f(u_m)\frac{dm}{du} du = \int_0^{\infty} f(u)\frac{l}{\pi a} du,$$

and, therefore, as $l \to \infty$,

$$\sigma_{yy} = \frac{qa}{l} - 4q \int_0^{\infty} \frac{l}{\pi a} \frac{\sin u \cos \frac{u}{a} x}{u} \times$$

$$\left( \frac{u \sinh u \sinh u - u \cosh u \cosh u - \sinh u \cosh u}{2u + \sinh 2u} \right) du. \quad (3.2)$$

The strain relaxation at the free surface is really of interest only for large $c$. It is appropriate, therefore, to take the limits $\frac{c}{a} \to \infty$ and $\frac{a}{u} \to \infty$, in which case equation 3.2 reduces to,

$$\sigma_{yy} \to \frac{2q}{\pi} \int_0^{\infty} du \frac{\sin u \cos \frac{u}{a} y}{u} \left[ 1 - \frac{y - c}{a} \right] \exp \left[ \frac{u - c}{a} \right].$$

Substituting, $w = c - y$, gives

$$\sigma_{yy} = \frac{2q}{\pi} \int_0^{\infty} du \frac{\sin u \cos \frac{u}{a} w}{u} \left[ 1 - \frac{w}{a} \right] \exp \left[ -\frac{u}{a} \right].$$

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The integral with respect to \( u \) is simple to evaluate and gives

\[
\sigma_{yy} = \frac{2aq}{\pi} \left\{ \frac{\arctan \left( \frac{x+w}{w} \right) - \arctan \left( \frac{x-w}{w} \right)}{2a} + \frac{w(a^2 + w^2 - x^2)}{((a-x)^2 + w^2)((a+x)^2 + w^2)} \right\}.
\]  

(3.3)

The same procedure can be carried out for the other stresses, and on the stresses for a tangential applied force. All the stresses derived in this way are similar in form to \( \sigma_{yy} \) of equation 3.3, where \( x \) is the distance, parallel to the surface, from the centre of the strained-layer and \( w \) is the perpendicular distance from the surface (positive \( w \) going into the material):

\[
\sigma_{xy} = \frac{2aq}{\pi} \left\{ \frac{2xw^2}{((a+x)^2 + w^2)((a-x)^2 + w^2)} \right\},
\]  

(3.4)

and

\[
\sigma_{xx} = \frac{2aq}{\pi} \left\{ \frac{\arctan \left( \frac{x-w}{w} \right) + \arctan \left( \frac{x+w}{w} \right)}{2a} + \frac{w(a^2 + w^2 - x^2)}{((a-x)^2 + w^2)((a+x)^2 + w^2)} \right\}.
\]

Figure 3.17 shows a contour plot of \( \sigma_{yy} \) and \( \sigma_{xy} \) together with similar plots obtained using the Fourier-series method. The agreement is very good: the stresses match to within 10% over most of the region shown. The difference in the stresses close to the surface arises because, as mentioned in section 2.3, the Fourier-series program is in error near the surface. Also, the Fourier-series calculation was for a block with dimensions of same order as the top-hat dimensions, which means that the close proximity of the free surfaces at \( x = \pm l \) will influence the stresses in the region of the applied force. This explains, therefore, the difference between the shears at larger distances from the centre of the layer.

Equations 3.3 and 3.4 provide analytic expressions for stress, and hence strains and displacements, where a strained-layer meets a free surface provided that \( c, l \) and \( y \) are very much larger than \( a \). The analytic expressions are much easier to employ than the summations and are exact. Further more, the analytic expressions can be used to find the functional forms for the stresses in certain circumstances. For instance, if \( x = 0 \) then expression 3.3 for \( \sigma_{yy} \) reduces to,

\[
\sigma_{yy} \rightarrow \frac{2}{\pi} g \left( \frac{w}{2a} \right)^{-1},
\]
Figure 3.17: Contour plots of stress obtained using the Fourier-series method and the Fourier-integral method. The top plots are from the Fourier-series method, the middle two are from the Fourier-integral method and those at the bottom show the difference between the two. The plots on the left show $\sigma_{yy}$ and those on the right show $\sigma_{xy}$.
and similarly the expression for $\sigma_{xy}$ can be reduced to,

$$\sigma_{xy} \rightarrow \frac{2}{\pi} q \left( \frac{w}{2a} \right)^{-2}.$$ 

These results can be compared to the expression derived by Faux using the Fourier-series method. He showed that, for large distances from the surface along $x = 0$,

$$\frac{\sigma_{xy}}{q} = K \left( \frac{w}{2a} \right)^{-1} \text{ where } K \approx 0.626.$$ 

Thus the correct constant is $\frac{2}{\pi}$ which is approximately equal to 0.636 and not 0.626.

In principle, a similar derivation to that above can be carried out for any functional form of stress imposed on the surfaces $y = \pm c$; although, of course, the integration required might be intractable. However, through the Green-function method, the stress field for an arbitrary boundary stress may be calculated in a more simple way.

The Green-function method is described in detail at the beginning of chapter 4. In order to apply this technique, the stress fields due to point forces acting normally and tangentially to a free surface are required.

A top-hat function of width $2a$ and height $q$ tends to a delta function if $2aq \rightarrow 1$ as $a \rightarrow 0$; therefore the stress field for a point force may be obtained by letting $2aq \rightarrow 1$ as $a \rightarrow 0$ in the stress field for a top-hat force. The stress field for a tangential top-hat force can be calculated in the same manner as that for the normal force above. If the appropriate limits are applied to these two stress fields the following stress distributions are obtained:

for the point normal force,

$$\sigma_{vv}^N = \frac{2}{\pi} \frac{y^3}{(x^2 + y^2)^2}, \quad \sigma_{sv}^N = \frac{2}{\pi} \frac{xy^2}{(x^2 + y^2)^2} \quad \text{and} \quad \sigma_{ss}^N = \frac{2}{\pi} \frac{y^2}{(x^2 + y^2)^2};$$

and for the point tangential force,

$$\sigma_{vv}^T = \frac{2}{\pi} \frac{xy^2}{(x^2 + y^2)^2}, \quad \sigma_{sv}^T = \frac{2}{\pi} \frac{y^2}{(x^2 + y^2)^2} \quad \text{and} \quad \sigma_{ss}^T = \frac{2}{\pi} \frac{x^3}{(x^2 + y^2)^2},$$

where $x$ is the distance from the point source parallel to the surface and $y$ is the perpendicular distance into the medium.

These point-force stress fields can be used as Green functions, described in Chapter 4, to obtain the stress field for other force distributions. For a normal applied stress $f(x)$ and
a tangential applied stress $g(x)$ the stress field will be:

$$\sigma(x, y) = \int_{-\infty}^{+\infty} \left\{ \sigma^N(x - x', y) f(x') + \sigma^T(x - x', y) g(x') \right\} dx', \quad (3.5)$$

where $\sigma^N(x, y)$ and $\sigma^T(x, y)$ refer to any one of the three possible stress components.

For example, the integration,

$$\int_{-\pi}^{\pi} q_\varphi N(x - x', y) dx' = \int_{-\pi}^{\pi} \frac{2q}{\pi} \frac{y^3}{((x - x')^2 + y^2)^2} dx',$$

reconstructs the $\sigma_{\varphi N}$ for a top-hat normal force given in equation 3.3.

In some cases the integration required in calculating the stress fields of other force distributions may be carried out analytically. However, the integration may often have to be numerical; in which case a 1-D integral is required for each $x, y$ coordinate. Whether or not calculating the stress field in this way is easier than using the Fourier-series method will depend on the forces being applied. For force distributions that are difficult to integrate, it is likely that the fewer integrations required for the Fourier-series method will mean it is more suitable than the Green-function method, and vice-versa.

The Fourier-integral method, therefore, provides an alternative way to calculate the stress distribution arising from an arbitrary applied force, and the extension to the point forces and Green-function method gives an even simpler technique for some problems.
Chapter 4

Green-function Method

Given the unfortunate complexity of the Fourier-series method for solving the problem of the buried-layer, another more simple technique is required. The Green-function method presented in this chapter is a simple way of obtaining analytic strain distributions about arbitrarily shaped buried-inclusions. Sections 4.1 and 4.2 develop the technique and in section 4.3 the results for a buried layer are presented.

Strain influences the electronic properties of III-V materials. The hydrostatic component of strain shifts the conduction-band and average valence-band energies, and the axial-strain component modifies the valence-band states at the valence-band maximum. The influence of the strain-relaxation of a buried layer on the layer’s electronic properties is discussed in section 4.4.

An introduction to the Green-function method can be found in most undergraduate textbooks on partial differential equations. The book by Williams (1980) gives a brief description.

4.1 The inclusion

The state of strain in a body is found by solving the differential equation 1.12. The Green’s function technique is a method of solving such equations. The way in which it is used
here involves considering a finite inclusion to be the superposition of an infinite number of infinitesimal inclusions.

The superposition of circular inclusions to model a rectangular inclusion, illustrated in figure 4.1, will inevitably leave some of the rectangle counted twice and some uncounted. However, as long as the total extra included material is equal to that of the rectangular inclusion, then, as the area of the circular inclusions tends to zero, the detail of the superposition is irrelevant.

Figure 4.1: The superposition of many small circular inclusions can approximate a larger inclusion of a different shape.

Equation 1.12 governs an elastic body with no internal sources of stress. For a body with internal sources the equation is modified to

$$\nabla^4 \Phi = f(r),$$  \hspace{1cm} (4.1)

where $f(r)$ is some function describing the source of the internal stresses.

Supposing we have some function $G(r, r')$ which satisfies

$$\nabla^4 G(r, r') = \delta(r - r'),$$  \hspace{1cm} (4.2)

then for all $r \neq r'$, $G(r, r')$ is a solution of the homogeneous equation.

However, $G(r, r')$ can be used to solve the non-homogeneous equation because

$$\nabla^4 \int_A G(r, r') f(r') dA(r') = \int_A \nabla^4 G(r, r') f(r') dA(r')$$

$$= \int_A \delta(r - r') f(r') dA(r') = f(r),$$  \hspace{1cm} (4.3)

where $A$ indicates integration over all space and $f(r)$ is non-zero only within the inclusion. Comparison of equations 4.1 and 4.3 shows that,

$$\Phi(r) = \int_A G(r, r') f(r') dA(r').$$  \hspace{1cm} (4.4)
Therefore a solution to equation 4.2 is required, where the delta function represents the source arising from an infinitesimal inclusion.

Fortunately, the stress field about an infinitesimal circular inclusion is easily obtained. The problem is simplified because it is a case of plane strain and because the solution must have circular symmetry. The Airy stress function therefore has the form, \( \phi(r) = \phi(r, \theta) = f(r) \), for which the general solution, from page 68 of Timoshenko (1970), is,

\[
\phi(r, \theta) = A \log |r| + B r^2 \log |r| + C r^4 + D. \tag{4.5}
\]

From this stress function, the radial and tangential stresses can be obtained. For a circular inclusion the stresses must be bounded both at the origin and, for an infinite medium, as \( r \to \infty \):

outside the inclusion,

\[
\sigma_{rr} = \frac{A}{r^2}, \quad \sigma_{\theta\theta} = -\frac{A}{r^2} \quad \text{and} \quad \sigma_{\theta r} = 0, \tag{4.6}
\]

and inside the inclusion,

\[
\sigma_{rr} = 2C, \quad \sigma_{\theta\theta} = 2C \quad \text{and} \quad \sigma_{\theta r} = 0. \tag{4.7}
\]

Hooke’s laws give the strains which can be integrated for the displacements: outside the inclusion,

\[
\epsilon_{rr} = A \frac{1 - \nu}{E} \frac{1}{r^2} \quad \text{and} \quad u_r = \int_r^\infty \epsilon_{rr} dr = A \frac{1 - \nu}{E} \frac{1}{r^2},
\]

and inside the inclusion,

\[
\epsilon_{rr} = \frac{2(1 + 2\nu)(1 - \nu)C}{E} \quad \text{and} \quad u_r = \int_r^0 \epsilon_{rr} dr = -\frac{2(1 + 2\nu)(1 - \nu)Cr}{E}.
\]

If the hole into which the inclusion is placed has a radius \( r_0 \) and the inclusion has a radius \( r_0(1 + \frac{\delta}{2}) \), then, to first order, the extra volume included is a fraction \( \delta \) of the volume into which it is placed. At \( r = r_0 \) there must be a discontinuity of radial displacement, \( \frac{\delta}{2} r_0 \), and continuity of radial stress at \( r = r_0 \), which gives a pair of simultaneous equations. These can be solved to find the constant \( A \) in equation 4.6, which gives

\[
A = \frac{E\delta r_0^2}{4(1 - \nu)^2}. \tag{4.8}
\]
The analysis considers the inclusions in two dimensions, obviously if a cylindrical inclusion was considered, the analysis would be identical and the extra volume per unit length would be equal to \( \delta \). If the constant of 4.8 is divided by the area of the inclusion, \( \pi r_0^2 \), one obtains the constant for the stress field per unit area of an inclusion with an area oversized by a fraction \( \delta \),

\[
A = \frac{E\delta}{4\pi(1 - \nu)^2}.
\]  

(4.9)

The constant of 4.9 is independent of \( r_0 \), the radius of the inclusion, and remains unchanged as \( r_0 \to 0 \) for the point inclusion. Therefore, replacing \( r \) by \( r - r' \) gives a Green-function, \( G(r, r') \), for the stress field of an infinitesimal inclusion centred at \( r' \):

\[
\sigma_{rr} = A \frac{1}{(r - r')^2}, \quad \sigma_{\theta\theta} = -A \frac{1}{(r - r')^2}, \quad \text{where} \ A = \frac{E\delta}{4\pi(1 - \nu)^2}
\]  

(4.10)

The Green-function, given above, can be used to reconstruct the stress field of the circular inclusion of radius \( r_0 \), and the result obtained is equal to that given in equations 4.6, 4.7 and 4.8. In a similar fashion to the derivation of the stress field, it is also possible to obtain the strain-field, displacement-field or stress-function for an infinitesimal inclusion; any of which can be used as a Green-function, and give the strain-field, displacement-field or stress-function respectively.

In principle the Green-function for the stress field can be used to construct the stress distribution of any arbitrarily shaped inclusion; although the integration of equation 4.3 might not always be possible analytically. In the following section the Green-function method is used to construct the stress field about a buried layer.

### 4.2 Buried layer

Using the Green’s function to calculate the stress field, \( \sigma^{\text{layer}} \), of the buried layer, shown in figure 4.2, requires the following integration:

\[
\sigma^{\text{layer}}(x, y) = \int_A G(r, r')f(r')dA(r'),
\]  

(4.11)
where \( f(r) = 1 \) for \( r \) inside the layer and \( f(r) \) is zero outside, giving the integral in cartesian coordinates,

\[
\sigma_{\text{layer}}(x, y) = \int_{-c}^{+c} \int_{-l}^{+l} G(x - x', y - y') \, dx' \, dy'. \tag{4.12}
\]

![Figure 4.2: Geometry of the buried layer.](image)

It is important to realise that there is an axial strain, \( \epsilon_{zz} \), present within the buried layer shown in figure 4.2. The Green’s function used for the layer must therefore be for an infinitesimal inclusion experiencing the same axial strain. This necessitates a small modification to the constant \( A \) for the Green-function derived in the previous section.

For an inclusion with a finite \( \epsilon_{zz} \), the radial strain is modified by the Poisson’s ratio effect,

\[
\epsilon_{rr} = 2\left(1 + \nu\right)\frac{(1-\nu)}{E} \left(C - \nu \epsilon_0\right) \tag{4.13}
\]

When 4.13 is used to calculate \( u_r \), and the boundary conditions are subsequently satisfied, the functional form of the stress field remains the same, but a different \( A \) is obtained,

\[
A = \frac{E \left(\frac{\delta}{2} + \nu \epsilon_0\right)}{2\pi (1 - \nu)(1 + \nu)},
\]

where \( \delta \) is equal to the fractional extra area of the inclusion, which, for a strained buried layer, is equal to \( 2\epsilon_0 \) and, therefore, for the buried layer,

\[
A = \frac{E \epsilon_0}{2\pi (1 - \nu)}. \tag{4.14}
\]
The integration of equation 4.12 is easy to perform in cartesian coordinates. Converting the stresses of the inclusion to cartesians:

\[ \sigma_{xx}^{\text{inc}} = A \frac{x^2 - y^2}{(x^2 + y^2)^2}, \quad \sigma_{yy}^{\text{inc}} = -A \frac{x^2 - y^2}{(x^2 + y^2)^2} \quad \text{and} \quad \sigma_{xy}^{\text{inc}} = 2A \frac{xy}{(x^2 + y^2)^2}. \]

Subsequently, performing the integration gives the stress field for a buried layer:

\[ \sigma_{xx}^{\text{layer}} = A \left\{ \arctan \left( \frac{l - x}{c - y} \right) + \arctan \left( \frac{l + x}{c - y} \right) \\ + \arctan \left( \frac{l - x}{c + y} \right) + \arctan \left( \frac{l + x}{c + y} \right) \right\}, \]

\[ \sigma_{yy}^{\text{layer}} = A \left\{ \arctan \left( \frac{c - y}{l - x} \right) + \arctan \left( \frac{c - y}{l + x} \right) \\ + \arctan \left( \frac{c + y}{l - x} \right) + \arctan \left( \frac{c + y}{l + x} \right) \right\} \]

and

\[ \sigma_{xy}^{\text{layer}} = \frac{A}{2} \left\{ \ln \left[ (l + x)^2 + (c - y)^2 \right] + \ln \left[ (l - x)^2 + (c + y)^2 \right] \\ - \ln \left[ (l - x)^2 + (c - y)^2 \right] - \ln \left[ (l + x)^2 + (c + y)^2 \right] \right\}, \quad (4.15) \]

where \( A \) is given by 4.14.

Note that, if the dimensions of the buried layer tend to those of an infinite strained-layer; that is \( \varepsilon \to \infty \); then the in-plane stress, \( \sigma_0 \), tends to the well known value of \( E\varepsilon_0/(1 - \nu) \).

The complexity of 4.15 can be reduced by a simple geometric interpretation presented later, in section 4.4, along with electronic structure calculations where it has particular implications.

The strain fields for the buried layer can be obtained from Hooke's laws. Again the strain in the \( x \)-direction must be accounted for and therefore the standard Hooke's laws for plane strain, without any axial strain, are modified to:

\[ \varepsilon_{xx} = \frac{1}{E} \left[ (1 - \nu^2)\sigma_{xx} - \nu(1 + \nu)\sigma_{yy} \right] - \nu \varepsilon_{zz}(x, y), \]

\[ \varepsilon_{yy} = \frac{1}{E} \left[ (1 - \nu^2)\sigma_{yy} - \nu(1 + \nu)\sigma_{xx} \right] - \nu \varepsilon_{zz}(x, y) \]

60
and

$$
\epsilon_{xy} = \frac{2(1 + \nu)}{E} \sigma_{xy},
$$

(4.16)

where $\epsilon_{zz}(x, y)$ is the strain in the $z$-direction as a function of position in the $x$-$y$ plane and is equal to $\epsilon_0$ within the layer and is zero outside.

The stress and strain fields presented above have been checked against the calculations performed by Faux et al. (1994) using finite-element analysis. The FEA results for a single buried layer with a 1% misfit, together with those using equations 4.15 and 4.16, are shown in figure 4.3.

Figure 4.3: Axial strain, $\epsilon_{xx}$, along the positive $z$-axis of a buried strained layer. Dots represent results from the finite-element calculation and the solid lines are results from the Green-function method. Both calculations used $E = 8.5 \times 10^{10}$Pa and $\nu = 0.32$ for GaAs taken from Fitzgerald (1993). The different lines are for aspect-ratios ($l:c$) of 40:1, 20:1, 10:1, 5:1, 2:1 and 1:1; the top line is for 40:1 and the bottom for 1:1. The finite-element package generated many more data points, but for comparison purposes only a few are shown.

In the worst case, the strains differ, in absolute value, by only 3%. These small differences almost certainly arise because of the limited size of the finite-element calculations.
The relaxation of a layer buried in a finite medium will be larger than that buried in an infinite medium because in the former case there is less material constricting the layer. As the aspect-ratio decreases, the difference in the results of the two methods increases because of the geometry used in the finite-element analysis. In the finite-element model, the aspect-ratio of the layers is changed by varying only the thickness of the layer; therefore, layers with low aspect-ratios are larger than those of high aspect-ratios. However, the layers are all buried in the same fixed amount of material. Thus, in the finite-element calculations, the layers with higher aspect-ratios have proportionately more material straining the layer, and, therefore, one would expect the longer and thinner layers to have a strain closer to that of the analytic calculations.

The case where \( c = l \) corresponds to a quantum wire with square cross-section and the results confirm that the strain is considerably relaxed in the cross-section. On average the strain in the \( x \) or \( y \) directions is about 0.09\( \varepsilon_0 \). In other words, for the value of Poisson's ratio used, strain relaxation ensures that less than 10% of any misfit strain remains across the short dimensions of the quantum wire.

The results, therefore, provide simple expressions for calculating stress, strain and displacement in rectangular buried layers in an infinite medium. These results have been published by Downes and Faux (1994).

### 4.3 Stress and strain fields of buried layers

Many buried quantum-well devices consist of quantum-well stacks with up to 20 separate quantum wells. The strain fields for single buried layers can be superposed to give the strain field of a stack. In this section, a stack of four compressive layers with aspect ratios of 1:400 is studied. The geometry of the four layers is shown in figure 4.4.

The strain fields about the layers is calculated using equations 4.15 and 4.16 and is shown in figure 4.5, for four separate cases.

In all four cases, the compressive layers have a 1% mismatch with the substrate. In the first, the four layers are separated by unstrained barriers of equal thickness. In the second
the barriers are still unstrained, but the separation between compressive layers is doubled. The third and fourth cases have identical geometry to the first two, but the barriers are tensilely-mismatched to the substrate by 1%.

Figures 4.5(a) and 4.5(b) show that structures with unstrained barriers suffer strain relaxation which extends a significant distance from the edge of each layer. This agrees with the previous calculations of relaxation by Faux and Haigh (1990), as does the slight modification to the strain distributions when the layers are in close proximity. Figure 4.5(c) shows that the strain-compensated stack, in which the tensile barriers are of the same thickness as the layers, contains compressive layers which retain their misfit strain over most of their length. Strain relaxation only occurs significantly over a distance of 2 layer thicknesses from the end of the layer. Figure 4.5(d) shows that the tensile barriers of double the layer thickness lead to strain in excess of the misfit in the compressive layers.

If the net strained material in the structures is measured in layer thickness multiplied by strain, then (a) and (b) have relative net strains of '+4' compared to '+1' for (c) and '−2' for (d). According to St. Venants principle the net strain relaxation should drop off at a similar rate for all four stacks because the dimensions of the layers are all approximately equal. The net strain in the four-layer stacks is smaller for (c) than for (d), which is in turn smaller than that for (a) and (b). Therefore, one would expect that, at a given distance from the facet, the strain in the layers of (c) would be less than that of (d), which would in turn be less than that of (a) and (b).
Figure 4.5: The strain in the $x$-direction, $\varepsilon_{xx}$, is shown for a variety of buried-layer stacks. The layers have dimensions $c = 1$ and $l = 400$, and the plots show the region $385 < x < 415$, $0 < y < 15$. The labels indicate absolute strain in $10^{-3}$. Compressive strains are shown as positive values in this figure in accordance with the convention used by band structure theorists.

Figure 4.6: The absolute strain, $\varepsilon_{xx}$, along the centre of the central strained layers shown in figure 4.5. The layers have dimensions $c = l = 400$, and the graph is for $350 < z < 400$. Compressive strains are shown as positive values in this figure in accordance with the convention used by band structure theorists.
A more detailed examination of the in-plane strain component is presented in figure 4.6. The results for stacks containing unstrained barriers confirm that relaxation has taken place over a considerable distance from the end of the layers. Over one eighth of the length of the layer $\epsilon_{zz}$ does not exceed 95% of the misfit. In the stack containing tensile barriers of thickness 2$c$, however, the strain is very close to 1% over the entire length of the layer. Tensile barriers of twice the layer thickness lead to over-compression in the compressive layers. It is clear that for a given structure it is possible to determine thicknesses and strains of barriers which would keep relaxation of the layers to a minimum.

4.4 Electronic structure

Strain influences the electronic properties of III-V materials. The hydrostatic component of strain, $\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$, shifts the conduction band and average valence band energies, while the axial-strain components, $\epsilon_{xx} - \epsilon_{yy}$, $\epsilon_{yy} - \epsilon_{zz}$ and $\epsilon_{zz} - \epsilon_{xx}$, modify the valence-band states at the valence band maximum\(^1\).

---

\(1\)When studying electronic structure the term 'axial strain' does not refer to strain along the axis of a buried layer, but instead to the three combinations of stresses mentioned in this sentence.
distances linking a given point to the corners of the layer. Figure 4.7 shows the geometry of the buried layer with the angles $\theta_a$ and $\theta_b$ and distances $d_1$ to $d_4$, which allow the stresses within the layer to be expressed as

$$\sigma_{zz} = \frac{\varepsilon_0 E}{1 - \nu} \frac{\theta}{2\pi}, \quad \sigma_{\nu\nu} = \frac{\varepsilon_0 E}{1 - \nu} \frac{2\pi - \theta}{2\pi} \quad \text{and} \quad \sigma_{\nu\gamma} = \frac{\varepsilon_0 E}{1 - \nu} \ln \left| \frac{d_1 d_4}{d_2 d_3} \right|,$$

where $\theta = \theta_a + \theta_b$. The stresses outside the layer are still given by equations 4.15.

When using Hooke's laws, the following strains are obtained:

$$\varepsilon_{zz} = \left( \frac{1 + \nu \theta}{1 - \nu} - \frac{2\nu}{2\pi} \right) \varepsilon_0, \quad \varepsilon_{\nu\nu} = \left( 1 - \frac{1 + \nu \theta}{1 - \nu} \right) \varepsilon_0$$

and

$$\varepsilon_{\nu\gamma} = \frac{\varepsilon_0 (1 + \nu)}{1 - \nu} \ln \left| \frac{d_1 d_4}{d_2 d_3} \right|.$$

These expressions reduce to the standard results for an infinite buried layer (where $\theta \to 0$ or $\theta \to 2\pi$) with the in-plane strain, $\varepsilon_{||}$, and strain perpendicular to the plane, $\varepsilon_{\perp}$, given by,

$$\varepsilon_{||} = \varepsilon_0 \quad \text{and} \quad \varepsilon_{\perp} = -\frac{2\nu}{1 - \nu} \varepsilon_0.$$

Equations 4.18 also show that $\varepsilon_{\nu\nu}$ is equal to $(2 - 4\nu)/(1 - \nu)\varepsilon_0$, and is constant and independent of position throughout the strained layer. This results in a constant conduction band-edge energy within the layer. Poisson's ratio is typically close to $\frac{1}{3}$ in III-V semiconductors, which means that $\varepsilon_{\nu\nu}$ is usually close to $\varepsilon_0$.

Equations 4.18 provide a simple pictorial means of estimating the strain distribution within a rectangular inclusion. The angle $\theta$ is an immediate indication of the deviation between the tetragonal strain and that which would be found in an infinite buried layer. By splitting $\theta$ into $\theta_a$ and $\theta_b$, the deviation can be viewed as having two separate contributions associated with each side of the inclusion.

Figure 4.8 shows contour plots of $\frac{\theta}{2\pi}$ as a function of position near the edge of buried layers with aspect ratios varying from 1:1 to 1:∞. There are marked differences between the four contour plots shown. Even when the ratio of the sides is 10:1 the values of $\theta$ are significantly different from those in the semi-infinite layer. In contrast, the contour
Figure 4.8: Contour plots showing lines of constant $\frac{\theta}{2\pi}$ in the upper right-hand corner of buried layers with varying aspect-ratio.

Figure 4.9: Contour plots showing lines of constant $\ln\left(\frac{d_2 \Delta}{d_1 \Delta_3}\right)$ in the upper right-hand corner of buried layers with varying aspect-ratio.
plots of $\ln \left| \frac{\partial d}{\partial d_3} \right|$ shown in figure 4.9 are of a similar form for all aspect-ratios. Again two separate contributions from each end of the inclusion can be identified because $\ln \left| \frac{\partial d}{\partial d_3} \right| = \ln \left| \frac{\partial d}{\partial d_2} \right| + \ln \left| \frac{\partial d}{\partial d_1} \right|$. However, because $\ln \left| \frac{\partial d}{\partial d_2} \right|$ drops off as $\frac{1}{x}$ for large distances, $x$, from the edge, the separate contributions rapidly decouple, and contour plots of $\ln \left| \frac{\partial d}{\partial d_3} \right|$ rapidly converge towards the result for the ends of an infinite layer.

The hydrostatic component of strain, $\epsilon_{\text{vol}}$, leads to a shift in the conduction band-edge energy, $E_c$, and the average valence-band edge energy, $E_v$, given by equation 1.15. It was shown above that $\epsilon_{\text{vol}}$ is constant and, therefore, the hydrostatic strain will lead to a rigid shift of the band energies.

Although the axial component of strain has no influence on the conduction band edge energy, it can significantly modify the valence band character. The 6 × 6 Luttinger-Kohn Hamiltonian, which includes the heavy-hole, light-hole and spin split-off band interactions, can be used to treat the valence bands. Expressed in a basis combining the ↑ and ↓ spin functions and spatial functions $X$, $Y$ and $Z$, the Luttinger-Kohn Hamiltonian is given by,

\[
H = \begin{pmatrix}
X \uparrow & 
\begin{bmatrix}
    p - q - \Delta & r - i\Delta & 0 & 0 & 0 & \Delta \\
    r + i\Delta & -2p + q - \Delta & 0 & 0 & 0 & -i\Delta \\
    0 & 0 & p - \Delta & -\Delta & i\Delta & 0 \\
    0 & 0 & -\Delta & p - q - \Delta & c + i\Delta & 0 \\
    \Delta & i\Delta & 0 & 0 & 0 & p - \Delta \\
\end{bmatrix}
\end{pmatrix}
\]  

where,

$$p = b \varepsilon_0 \left( \frac{1 + \nu}{1 - \nu} \right), \quad q = b \varepsilon_0 \left( \frac{1 + \nu}{1 - \nu} \right) \frac{3\theta}{2\pi}, \quad r = \sqrt{3}d\varepsilon_{xy} \quad \text{and} \quad \Delta = \frac{E_{SO}}{3},$$

and where $b$ and $d$ are the (001) and (111) axial deformation potentials, and $E_{SO}$ is equal to the spin-orbit splitting for zero strain. The diagonal terms involving $p$ and $q$ were found by substituting the strains of equations 4.18 into the general expressions for the matrix elements given in 1.15.

Equation 4.20 can be solved to find the energy and character of the zone-centre valence states as a function of position within the rectangular inclusion. It is, however, also instructive to consider the case where the strain terms are small compared to the spin-orbit splitting interaction $\Delta$. In this case the strain-induced interaction between the heavy-hole and light-hole bands with the spin split-off band can be ignored and, rewriting the
Figure 4.10: Contour plots showing lines of constant valence band-edge energy (eV) in the upper right-hand corner of buried layers with varying aspect-ratio.

Hamiltonian in a basis of heavy-hole and light-hole states, the $4 \times 4$ zone-centre Hamiltonian matrix splits into two independent $2 \times 2$ matrices,

$$H = \begin{pmatrix} HH & L \bar{H} \\ L H & \bar{L} \end{pmatrix} = \begin{pmatrix} -\frac{p}{2} & -\frac{\sqrt{3}p}{2} + \frac{q}{\sqrt{3}} \pm i\frac{p}{\sqrt{3}} \\ -\frac{\sqrt{3}p}{2} + \frac{q}{\sqrt{3}} + i\frac{p}{\sqrt{3}} & \frac{p}{2} \end{pmatrix}. \quad (4.21)$$

From equation 4.21, the band edge energies at the valence band maximum in the rectangular wire vary with $\theta$ and $\epsilon_{x y}$ as,

$$E = \pm \left\{ \frac{p^2}{4} \left[ 4 - \frac{6\theta}{\pi} + \frac{3\theta^2}{\pi^2} \right] + d^2 \epsilon_{x y}^2 \right\}^{\frac{1}{2}}. \quad (4.22)$$

Figure 4.10 shows the variation of the valence band maximum with position in layers of varying cross-sectional aspect-ratio, for a layer with $\epsilon_0 = 1\%$, $\nu = \frac{1}{3}$, $b = -1.6\text{eV}$ and $d = -5.0\text{eV}$, appropriate for GaAs.

The axial strain at the centre of the square wire, $\epsilon_{x x} = \epsilon_{y y} - \frac{1}{2}(\epsilon_{x x} + \epsilon_{y y})$, is exactly half that in an infinite strained-layer, so the shift in band-edge energy there, $+\frac{p}{2}$, is also half that found in an infinite layer, $+p$. For each of the layers shown in figure 4.10, the valence-band
energy rises to a maximum in the corners of the wire because of shear strain. This leads to potential wells for holes in the corners of the layer. The dimensions of the strain-induced well scales with the size of the inclusion, and the depth of the well scales with the lattice mismatch $\varepsilon_0$.

4.5 Discussion

The Green-function method for calculating stress fields about buried-inclusions is presented in this chapter. The method is subsequently used to calculate the stress field about a buried strained-layer and the results agree very well with a previous finite-element analysis. This simple method can be used to calculate the stress fields about other buried inclusions and it is not necessarily limited to treating only semiconductor structures, although the analysis of triangular and crescent-shaped quantum wires would be particularly interesting.

Section 4.4 discusses the electronic properties of the buried layer, of which the most significant points follow. The hydrostatic pressure is constant throughout the buried layer and, therefore, the band gap is constant. The high shear strains at the corners of the layer modify the valence band and result in potential 'wells' for holes at the corners. These two effects may affect the operation of devices based on such layers. Grundmann et al. (1994) discussed the symmetry splitting of the hole ground-state wave-function in crescent shaped quantum wires, and also the influence of the piezoelectric effect. In a fuller analysis of the electronic and piezoelectric properties, similar effects may be observed for the corners of buried layers.
Chapter 5

Critical Thickness

5.1 Introduction

Strained layers relax plastically above the critical thickness through the nucleation and propagation of dislocations. The theoretical work on critical thickness can be divided into two types: that which considers the energy equilibrium and that which considers dislocation nucleation processes. Historically the equilibrium theories appeared first in the literature which is why, perhaps, they seem to have been dominant.

Van der Merwe (1963a, 1963b) first introduced the idea of a critical thickness, but it was Matthews and Blakeslee who established an equilibrium theory in 1974 (referred to from hereon as 'Matthews'). He equated the force tending to move a threading dislocation, which creates a segment of misfit dislocation, to the line tension of the misfit dislocation.

A dislocation which is present in the substrate, and subsequently threads through each monolayer as a strained layer is grown, is known as a threading dislocation. The dislocation is therefore already present in the layer before any relaxation occurs, and no nucleation processes need be considered. One of the principal strain-relieving dislocations for layers grown on the (100) surface is the 60° partial dislocation. Figure 5.1 shows its geometry and how it may glide through a layer introducing a dislocation dipole with a burgers vector component that acts to relieve strain. The force tending to move the threader is equal to the
strain energy itrelieves per unit distance it moves, and the line tension of the dislocation is the energy required to create a unit length of dislocation line. Therefore, the Matthews procedure of balancing forces is an energy equilibrium method.

There have been subsequent refinements to work on the single threader. People and Bean (1985) realised that the standard Matthews model does not consider dislocation nucleation, it considers only the propagation of threaders already present. They performed a calculation using the creation energy of half-loops of dislocation with radii equal to the layer thickness. Their critical thickness recorded good agreement with experiment which led to its frequent citation. Hu (1991) later pointed out that the coincidence of their analysis with experiment was because of the use of an 'areal' energy density which corresponded to an array of dislocations with a density that would completely relax the layers. He showed that they had equated the energy of this dislocation array with the energy of a strained layer, which is not the criterion for obtaining the critical thickness for the onset of relaxation. He proposed that experimentally-observed critical thicknesses much larger than the Matthews prediction must arise due to supercritical behaviour, and speculated that the supercritical layers break down by the sudden and catastrophic nucleation of dislocations. He suggested that strain...
Figure 5.2: The compound array, comprised of two types of dislocation with different Burger's vectors, can be energetically more stable than a more simple array. The figure is taken from Willis (1991).

relief would in practice more often occur by the gradual introduction of dislocations beyond the Matthews critical thickness.

In order to treat this gradual introduction of dislocations and to obtain a critical thickness for a particular density of strain-relieving dislocations, the energy of dislocation arrays is required. When considering arrays of dislocations one must account for the interaction energies. Dislocations with like-sign Burger's vectors usually repel one another; therefore, the energy per dislocation in an array of many like-sign dislocations is normally higher than that of a single dislocation.

The energy of a periodic array in an uncapped layer has been calculated by Willis et al. (1990, 1991a). The analysis has been extended to capped layers [Willis et al. (1991b)], where it was demonstrated that the energy of a compound array, shown in figure 5.2, could be energetically more favourable than a simple array, because adjacent dislocations with different Burger's vectors can interact in a way which reduces the total energy. The extension to the non-periodic array, reported in 1993 by Jain et al., gave an equilibrium theory that made predictions of the most energetically-favourable dislocation density, with a realistic distribution, for a given strain and layer thickness.

All the equilibrium theories, however, have shortcomings. They do not consider dislocation nucleation; instead they assume there are already sufficient threaders present for the relaxation. A typical dislocation density for a substrate is between $10^2 \text{ cm}^{-2}$ and $10^5 \text{ cm}^{-2}$, and densities of up to $10^9 \text{ cm}^{-2}$ are required to account for the relaxation observed [Beanland (1992)]. Therefore, it is clear that although equilibrium theories can predict a
The process requires dislocations to climb to the surface. Maximum relaxation and the minimum thickness at which relaxation can occur, they cannot predict the degree of relaxation actually observed.

Hagen and Strunk (1978) proposed a nucleation model, the Hagen-Strunk model, which involves two intersecting dislocations lying in the interface plane interacting with each other, according to figure 5.3. This mechanism will work in thin layers where the surface can attract the dislocation sufficiently to cause climb, but in thicker layers it is unlikely. The model was in part proposed to explain a particular dislocation configuration seen in relaxed layers, but this is more easily and better explained by simpler dislocation interactions.

Frank-Read multiplication, shown in figure 5.4, together with spiral sources were suggested by Beanland (1992). This does not leave a tell-tale dislocation configuration, but it does require layer thicknesses several times larger than the equilibrium critical thickness to operate. Relaxation is often observed to set in at thicknesses higher than critical, which is good evidence for the occurrence of Frank-Read or similar multiplication. Other nucleation processes, such as half-loops extending from the surface and nucleation from defects at the interface [Vignaud and Di Persio (1994)], have been suggested. However, it is accepted that glide mechanisms, like the Frank-Read source, are much more likely than those requiring climb [Jesser (1994)].

In order to predict the critical thickness for nucleation from a Frank-Read source it is necessary to calculate the layer thickness at which the glide shown in figure 5.4 can
occur. This is determined in the same way as Matthews critical thickness for the glide of a threader. Unfortunately, the way in which the core is treated when calculating the self-energy of dislocations gives rise to two ‘adjustable’ parameters, the core-radius and the core-energy. These two parameters, together with any other energy corrections (surface relaxation for uncapped layers and, for the screw component, the energy associated with the surface step) mean that the predictions of a given theory are not certain. To emphasise this point, the critical thickness predicted by the original Matthews theory is shown in figure 5.5 for a variety of core-radii taken from the literature. In fact, it can be seen that for low strains, two critical thicknesses are predicted, but for high strains no prediction is made. Such behaviour is not physical and means the model is not useful at high strains of interest to device designers.

The problem is further compounded by a large variety of experimentally predicted critical thicknesses. Data on plastic relaxation in strained layers has been gathered using a variety of techniques and criteria: some looking for the relaxation of strain, some observing the nucleation of dislocations, and others looking for loss in device performance. The techniques have widely varying resolution of dislocations and strain, which means experimental data can be gathered which would apparently fit any of the theories [Fritz (1987)].

Clearly there is a difficulty facing device designers who need to know, for a given
Figure 5.5: The critical thickness predicted by Matthews as a function of layer misfit, plotted for a pure edge dislocation with three different core-radii. All material parameters, except for Poisson’s ratio, cancel. The plot is for $\nu = \frac{1}{3}$ which is a value typical of most semiconductors.

strain, the thickness up to which a layer is stable. The equilibrium theories can predict the critical thickness for the first and subsequent dislocations, although they are subject to large uncertainties due to the core and other energies, and do not behave realistically at high strains. Meanwhile, layers which may be above critical thickness can appear stable because dislocation multiplication mechanisms are not operating.

The work presented in this chapter is concerned with the unrealistic behaviour of the equilibrium theories and will attempt to remove some of the uncertainty associated with the core.

5.2 Early equilibrium theory

The original Matthews theory of 1974 involves balancing the energy required to create a unit length of dislocation, known as the line tension, against the strain energy relieved by its presence. The layer thickness at which these two competing energies are equal is the Matthews critical thickness. The result relies on calculating these energies correctly. The analysis is easier for pure misfit dislocations with the geometry of the $60^\circ$ mixed added...
later, therefore edge dislocations are considered first.

The strain energy per unit length, $\Delta E_{rel}$, relieved by the presence of a pure edge dislocation dipole of Burger's vector $b$, in a layer of thickness $h$ and strain $\varepsilon$, is

$$\Delta E_{rel} = \sigma_0 bh = \frac{E}{(1 - \nu)} bh \varepsilon_0,$$  \hspace{1cm} (5.1)

where $E$ is the Young's modulus of the material and $\nu$ is the Poissons ratio. However the line tension of a dislocation is not deduced so easily.

The line tension is calculated usually by considering a dislocation in a continuous elastic medium. Mathematically an edge dislocation can be described as a line extending from the dislocation to infinity, along which there is a discontinuity of displacement equal to the Burger's vector. Figure 5.6 shows how the dislocation can be pictured physically. A hole has been drilled and a cut made to infinity. The surfaces of the cut have then been parted by the Burger's vector and rigid material inserted.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5.6.png}
\caption{A single edge-dislocation is modelled as a displacement equal to the burgers vector along a cut extending from a drilled hole, known as the core, to infinity, or the edge of the material.}
\end{figure}

The stress field about the mathematical edge dislocation can be obtained by finding a solution to equation 1.12 subject to appropriate boundary conditions. In polar coordinates these boundary conditions are, for the discontinuity lying along $\theta = 0$:

(a) $u \to 0$ as $r \to \infty$.

(b) $u$ is continuous everywhere except at $\theta = 0$ where $u(r, \theta^+) = +\frac{1}{2}b$

and $u(r, \theta^-) = -\frac{1}{2}b$

(c) $u$ is finite
The stresses in cylindrical polars, which are discussed in more detail by Cottrell (1953), are

\[
\sigma_{rr} = \sigma_{\theta\theta} = -D \frac{\sin \theta}{r} \quad \text{and} \quad \sigma_{r\theta} = D \frac{\cos \theta}{r} \quad \text{for} \ r > r_0 \quad \text{and where} \ D = \frac{\mu b}{2\pi(1 - \nu)},
\]

(5.2)

where it should be noted that the singularity as \( r \to 0 \) is avoided by introducing the cut-off radius, \( r_0 \), of the drilled hole.

Equations 5.2 can also be expressed in cartesians,

\[
\sigma_{xx} = -D \frac{y(3x^2 + y^2)}{(x^2 + y^2)^2}, \quad \sigma_{yy} = D \frac{y(x^2 - y^2)}{(x^2 + y^2)^2} \quad \text{and} \quad \sigma_{xy} = D \frac{x(x^2 - y^2)}{(x^2 + y^2)^2},
\]

(5.3)

where \( D \) is as in equation 5.2 and where \( x^2 + y^2 > r_0^2 \).

The line tension is equal to the strain energy stored in the stress field of the dislocation. Equation 1.13 gives a volume integral for the strain energy which, in this case, can be reduced to an area integral because the dislocation stress field is a state of plane strain. Use of the divergence theorem can further reduce this area integral to a line integral:

\[
\Delta E_{\text{line}} = \frac{1}{2} \int_A \sigma_{ij} \epsilon_{ij} \, dA = \frac{1}{2} \int_S (\sigma_{ij} n_j) u_i \, dS = \frac{1}{2} \int_S (\sigma_{ij} n_j) b_i \, dS,
\]

(5.4)

where \( A \) and \( S \) are indicated in figure 5.6.

In the Volterra model of the dislocation, the line integral corresponds to the work done against the stress field in moving the cut apart by the Burgers vector.

Evaluating the line integral using equation 5.2 requires the use of both an internal cut-off radius, \( r_0 \), and an external cut-off radius, \( r_1 \). Both cut-off radii are required to bound the integral. The inner cut-off radius maintains a finite stress as \( r \to 0 \), and the outer cut-off radius is required because the stress drops off slowly as \( \frac{1}{r} \). The internal cut-off radius is justified by noting that both Hooke's law and linear elasticity are not valid close to the dislocation core. The use of the external cut-off radius is reasonable because real crystals are not infinite and, even within a single crystal, other defects or surfaces will disrupt the stress field at large distances.

The line tension is, therefore,

\[
\Delta E_{\text{line}} = \frac{\mu b^2}{4\pi(1 - \nu)} \ln \left| \frac{r_1}{r_0} \right|
\]

(5.5)
Even though both \( r_0 \) and \( r_1 \) appear in only the In term, their choice influences the value of the line tension given by equation 5.5. Given the different values of \( r_0 \) cited in the literature, the value of the line tension may vary by a factor of 2 (Freund (1990) quotes \( r_0 = \frac{b}{4} \) and Cottrell (1953) suggests \( r_0 \) should be equal to a few \( b \)).

When Matthews considered a threading dislocation extending in a single capped layer, which will create a dislocation at both interfaces, he assumed that the presence of one dislocation would limit the stress field of the other to within a radius equal to the layer thickness. He chose \( r_0 \) equal to the magnitude of the Burgers vector and he obtained an expression for the critical thickness,

\[
\frac{h_c}{b} = \frac{1}{4\pi(1 + \nu)} \ln \left| \frac{h_c}{b} \right|.
\]

This result is flawed because it gives two solutions for the critical thickness at low strains and no solutions for strains greater than a critical value \( \epsilon_c \) given by

\[
\epsilon_c = \frac{1}{4\pi(1 + \nu)} e, \quad (5.7)
\]

where \( e \) is Euler's number. This means \( \epsilon_c \approx 2.2\% \) for \( \nu = \frac{1}{3} \).

### 5.3 Area integration versus line integration

It is the problems associated with evaluating the line integral which appear to cause the errors in Matthews analysis. In particular, it is not clear how to deal with the influence of one dislocation core on the core of the other. Strictly speaking, the line integral should be evaluated around both cores using the stress field of both dislocations, whereas in the literature it is assumed that one dislocations core does not exist when evaluating the line tension of the other dislocation.

Rather than using the divergence theorem to convert to a line integral (or calculating the strain energy by evaluating the work done in setting up the strain field), it is possible to calculate the strain energy as an area integral. When carrying out the area integration it is easy to be specific about the region over which the integral should be evaluated.
Figure 5.7: An edge dislocation dipole. The dislocations are separated by $h$ and have opposing Burger's vectors.

Although the strain energy about a single dislocation with a core radius but without an external cut-off radius is unbounded, the energy of two dislocations, with opposite Burger's vectors and separated a distance $h$ (a dislocation dipole), is finite. At large distances the strain fields tend to cancel in a manner similar to that of the electric fields of the point charges in an electric dipole.

It is possible to superpose the strain fields of a strained layer and a dislocation dipole, and calculate the energy of the combined system. This energy can then be compared to that of the strained layer with no dislocations. The layer thickness at which the two energies are equal is the equilibrium critical-thickness. If the core radius and dislocation stress fields are the same as those used in the line integration, then the predictions of critical thickness should be equal.

Without first converting to a line integral, the area integral cannot be carried out analytically; therefore, the integration must be carried out numerically. This is fortunate because this means one must be entirely specific about the treatment of the cores.

The stress field of the dipole shown in figure 5.7, with an inter-dislocation distance of $h$ positioned at the origin, obtained by superposing the stress field of two dislocations of opposing Burger's vectors and expressed in cartesian coordinates, is

$$
\sigma_{xx}^{dist} = \frac{Gb}{2\pi(1-\nu)} \left\{ \frac{(y - \frac{h}{2})(3x^2 + (y - \frac{h}{2})^2)}{(x^2 + (y - \frac{h}{2})^2)^2} - \frac{(y + \frac{h}{2})(3x^2 + (y + \frac{h}{2})^2)}{(x^2 + (y + \frac{h}{2})^2)^2} \right\},
$$
Figure 5.8: The separate regions used to perform the area integration are shown. The important feature is the increased fineness of the mesh near the centre of the dipole. The integration need only be performed over the half-space because of symmetry.

\[
\sigma_{yy}^{\text{disl}} = \frac{Gb}{2\pi(1 - \nu)} \left\{ \frac{(y + \frac{h}{2})(x^2 - (y + \frac{h}{2})^2)}{x^2 + (y + \frac{h}{2})^2} - \frac{(y - \frac{h}{2})(x^2 - (y - \frac{h}{2})^2)}{x^2 + (y - \frac{h}{2})^2} \right\}
\]
and

\[
\sigma_{xy}^{\text{disl}} = \frac{Gb}{2\pi(1 - \nu)} \left\{ \frac{x(x^2 - (y + \frac{h}{2})^2)}{x^2 + (y + \frac{h}{2})^2} - \frac{x(x^2 - (y - \frac{h}{2})^2)}{x^2 + (y - \frac{h}{2})^2} \right\},
\] (5.8)

and the stress field of a strained layer is

\[
\sigma_{xx} = \sigma_0, \quad \sigma_{yy} = 0 \quad \text{and} \quad \sigma_{zz} = \sigma_0, \quad \text{where} \quad \sigma_0 = \frac{E \varepsilon_0}{1 - \nu}.
\] (5.9)

The integration of this function efficiently poses a problem because of the singular nature of the fields at the core. Obtaining an accurate value of the energy near the core requires a very fine mesh, whereas integrating over a large region in order to approximate infinity requires a much coarser mesh. For a one-dimensional integral it is easy to modify the step size according to the rate of change of the integrand but, for a two-dimensional integral, the matching of the elemental areas correctly makes this more difficult. So instead of a continuous change in elemental area, the integration is carried out with differently sized elemental-areas in different regions according to figure 5.8.

The Simpson rule for evaluating the integral was tested, but the extra calculation involved for each point means that, although convergence with respect to number of mesh points is faster, the real time taken to converge is more than that of integrating by the
Convergence was checked both as the total integration area increased and as the fineness of the mesh increased. Figure 5.9 shows the value of the predicted critical thickness as a function of area size and number of mesh points. It can be seen that beyond $10^7$ mesh points and for areas larger than $10^4 h_c^2$ the predicted numerical value has converged to within a few percent of the final value. The results shown in figure 5.9 were for a very low value of $h_c$ for which the convergence was hardest to obtain; thus approximately $10^7$ mesh points and an area of approximately $10^4 h_c^2$ are used for all the calculations of $h_c$.

The energy outside the integration region $E_{r>r_{\text{max}}}$ can be estimated by noting that, for $\frac{r}{h} \approx \frac{h}{h} \gg 1$, terms in $h^2$ can be ignored. This leads to a simplified expression for the dipole stress field, which, in the absence of the strained layer, can be integrated analytically to give

$$E_{r>r_{\text{max}}} \approx \frac{\pi (72 + 16 \nu^2) \mu + 16E \left( \frac{\mu bh}{2\pi(1-\nu)r_{\text{max}}} \right)^2}{2\varepsilon\mu}.$$

For an area of $\approx 10^4 h^2$, $r_{\text{max}} \approx 160h$ therefore,

$$E_{r>r_{\text{max}}} \approx 10^{-12} \text{ Jm}^{-1} \text{ or } 10^{-6} \text{ eV/Å}.$$
the order $10^{-8}$ $\text{J m}^{-1}$ or $10^{-2}$ $\text{eV/Å}$. The energy excluded from the calculation is at least four orders of magnitude smaller than that included and it can, therefore, be ignored safely.

After making a reasonable guess at the critical thickness, the Newton-Raphson method can be used to obtain convergence to the real value. Figure 5.10 shows a plot of the difference in energy of the system with and without the dislocations, and the zero which the Newton-Raphson method selects. The results, shown in figure 5.11, were taken after convergence to within 0.1 burgers vectors of the true value.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure5_10}
\caption{The energy difference between a strained layer with and without a strain relieving dislocation dipole as a function of layer thickness, for a strain of 1%; and with $\nu = \frac{1}{3}$, $E = 8.5 \times 10^{10}$ $\text{Nm}^{-2}$ and $G = \frac{E}{2(1+\nu)}$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure5_11}
\caption{The results of the numerical calculation, with the critical thickness in Burgers vectors, are shown as circles along with the analytic predictions of equation 5.6. Poisson's ratio is $\frac{1}{3}$, and for the numerical calculation $E = 8.5 \times 10^{10}$ $\text{Nm}^{-2}$ and $G = \frac{E}{2(1+\nu)}$.}
\end{figure}

The results are single-valued and make predictions for strains up to 10%. This contrasts with the results obtained by line integration which are double valued.

5.4 Modified integration limits in the equilibrium theory

In order to understand the error in the equilibrium theories it is useful to consider there to be two types of dislocation model for the dislocation dipole studied in section 5.3: the
Figure 5.12: The additional material of the Volterra model, (a), is shorter than that of the mathematical model, (b), for an equal separation of the core centres. In the Volterra model the two core radii must be subtracted from $AB$ to obtain the length of the material added, whereas in the mathematical model the core radii do not need to be subtracted.

Volterra model in which holes are drilled and cuts made, and the mathematical model which involves a simple discontinuity of displacement. If an equilibrium theory is to give realistic results, then it is necessary that the dislocation model is applied correctly. By considering these two types of dislocation model, it is possible to indicate points in the analysis where mistakes might occur and, therefore, avoid such mistakes.

In the Volterra model, shown in figure 5.12(a), a pure edge dislocation is formed by drilling two holes and making a cut between them. The cut is subsequently parted to allow the insertion of additional material and, therefore, the model represents extra material between the edges of the two drilled holes.

The mathematical model, shown in figure 5.12(b), for a similar dipole, is simply a line of discontinuity of displacement equal to the burgers vector. It does not explicitly represent any extra material, but can be considered to model additional material along all of the line of discontinuity.

In order to calculate the energy of a dipole one needs to know the stress field about it.
The stress field of the mathematical model is well known, but in order to calculate a finite energy one must cut a line integration short of the singularities at both ends of the line of discontinuity. In stopping short of the singularities, the length of additional material is reduced to a distance between the two cut-off radii. If the line integration of equation 5.4 is carried out around cut-off radii of both dislocations this problem is overcome, but in the literature this has not been done.

On the other hand, the Volterra model, which is usually assumed to have the same stress field as the mathematical model, will naturally stop short of any singularity at the cores. In summary, the mathematical model represents additional material along the line of discontinuity between the internal and external cut-off radii, and the Volterra model represents material added between the edges of the two drilled holes.

Matthews theory of 1974 applies a model which represents the addition of a length $h - r_0$ of material because he sets the external cut-off radius $r_1$ equal to $h$ in the mathematical dislocation model. However, this is taken to relieve the strain associated with material stretching across the whole layer. Matthews therefore compares the energy associated with a length $h - r_0$ to that associated with a length $h$; this works well for $h \gg r_0$, but as $h \rightarrow r_0$ it leads to error. This is the reason for the poor behaviour of Matthews theory at high strains.

If a dipole that represents the addition of a length $h$ of material is introduced, by setting $r_1 = h + r_0$, so that the integration limits in equation 5.4 become $r_0$ and $h + r_0$, then following the usual analysis the critical thickness is given by

$$\frac{h_c}{b} = \frac{1}{e \frac{1}{4\pi(1+\nu)}} \ln \left| \frac{h_c}{b} + 1 \right|. \quad (5.11)$$

This is shown in figure 5.13 alongside the results of the numerical calculation. It is clear that this very small modification to the analysis achieves realistic predictions agreeing closely with those obtained by integrating numerically over an area.

The match is not exact because the models in the analytic and numerical calculations are not identical. In the numerical area integration the total strain energy of the mathematical dipole is found, except for the energy within $r_0$ of the dislocations. In the analytic calculation the strain energy of the Volterra dipole is evaluated using an inner cut-off radius of $r_0$ and
Figure 5.13: The critical thickness, in Burgers vectors, for an edge dislocation, predicted by the Matthews theory with modified integration limits is shown along side the results of the numerical calculation. Poisson’s ratio is $\frac{1}{3}$, and for the numerical calculation $E = 8.5 \times 10^{10}$ Nm$^{-2}$ and $G = \frac{E}{2(1+v)}$.

an outer cut-off radius of $h + r_0$. Although this approximates additional material equal in length to the layer thickness, the correct calculation is different. The line integration should be carried out, for each dislocation, along the paths shown in figure 5.14. Matthews and Blakeslee (1974) evaluates the contribution associated with $A'B, CD', EF'$ and $G'H$ and approximates the contributions from $BC$ and $HE$, but ignores $DA$ and $FG$. Freund (1990) later calculated exactly the contributions from $BC$ and $FG$, but still ignored $DA$ and $EG$. If the integration is carried out along $A''BCD''$ and $F''EHG''$ the approximation to the integration along $ABCD$ and $EFGH$ is better than $A'BCD'$ and $F'EHG'$, but is still in error as the difference between the results this predicts and those of the numerical area integration shows. The analysis using the paths $A''BCD''$ and $F''EHG''$, from here onwards, will be referred to as the ‘modified equilibrium theory’.

5.5 Extensions to the modified equilibrium theory
The principal strain-relieving dislocation for growth on \{100\} surfaces is the 60° mixed dislocation with Burgers vectors \( \frac{a}{2} < 110 > \), which is illustrated earlier in figure 5.1. This has a screw component and an edge component, of which the edge component can be further resolved into a component which relieves strain and one which does not. In order to evaluate the line tension of a dislocation with this Burger's vector one needs the stress field about a screw dislocation:

\[
\sigma_{zz} = -\frac{\mu b \sin \theta}{2\pi r}, \quad \sigma_{\theta z} = \frac{\mu b \cos \theta}{2\pi r} \quad \text{and} \quad \sigma_{\theta 0} = \frac{\mu b}{2\pi r}. \quad (5.12)
\]

The line tension of a single dislocation, using the physical model with the modified integration limits, is given by

\[
\Delta E_{\text{line}} = \frac{1}{2} \int_{L} \sigma_{ij} n_j u_i dL, \quad (5.13)
\]

where \( L \) extends a distance \( h \) from the edge of the core of the dislocation.

For the general case, where the Burgers vector makes an angle of \( \alpha \) to the dislocation line, the line tension is

\[
\Delta E_{\text{line}} = \frac{1}{2} \int_{r_0}^{h+r_0} \mu b \sin \alpha \frac{1}{2\pi(1-\nu)} \frac{1}{r} \left( \frac{\mu b}{2\pi r} \frac{1}{r} \right) dr = \mu b^2 \frac{1-\nu^2 \cos^2 \alpha}{4\pi} \ln \frac{h}{r_0} + 1. \quad (5.14)
\]

For a capped layer with a dislocation at both interfaces, twice this line tension can be equated to the energy relieved per unit length of the dislocation, where now only the
Figure 5.15: The critical thickness, in Burgers’ vectors, predicted by integrating over area for the energy and by the usual line integration with the modified limits (equation 5.16) are shown for a pure edge dislocation and for the $60^\circ$ dislocation. Both $\alpha$ and $\lambda$ are equal to $60^\circ$ and Poisson’s ration is equal to one third.

component $b \cos \lambda$ relieves strain and where $\lambda$ is the angle the edge component of the Burgers vector makes with the layer interface,

$$\Delta E_{\text{line}} = 2\mu \frac{1 + \nu}{1 - \nu} b \cos \lambda \kappa;$$

which gives the critical thickness,

$$\frac{h_c}{b} = \frac{1}{\epsilon} \frac{1 - \nu^2 \cos^2 \alpha}{4\pi(1 + \nu) \cos \lambda} \ln \left| \frac{h_c}{b} + 1 \right|.$$

The critical thickness can again be calculated by integrating over the area for the total energy of the system. Figure 5.15 shows the analytic curve of equation 5.16 and the numerical results of the area integration for the $60^\circ$ dislocation and for the pure edge. Once again the results match closely.

### 5.6 Energy corrections

#### 5.6.1 Integrating around the core

In the Volterra model of the dislocation the stress field of the mathematical model is assumed. The stress at the edge of the drilled holes is therefore not equal to zero. A traction
exists on the cylindrical surface of the holes which maintains the stress field outside. As the surfaces of the cut between the holes are parted, the surfaces of the drilled holes must also be displaced. Moving the surfaces of the holes requires energy which must be accounted for. In the mathematical model this is the energy associated with the integration along the paths $BC$ and $EG$ of figure 5.14. Bullough and Foreman (1963) and Freund (1990) calculated this integral,

$$\frac{1}{2} \int_{-\pi}^{+\pi} \sigma_{ij}^\infty r_j^0 u_i^\infty r_0 d\theta = -\frac{\mu b^2(1 - 2\nu)}{16\pi(1 - \nu)^2} \text{ for } r_0 = b,$$

(5.17)

where $\sigma_{ij}^\infty$ and $u_i^\infty$ are the stress and displacement fields associated with a dislocation in an infinite medium.

### 5.6.2 Non-crystallinity at the core

At the core of a dislocation the material is not crystalline. There is energy associated with dangling bonds and with strain in bonds that are not broken but are greatly deformed. Most semiconductors used in strained layers are alloys; therefore, the energy of the bonding configuration of the core depends on the types of atoms within the core. In order to calculate the core energy correctly one needs to resort to an atomic scale simulation similar to that of Hansen (1994) or Ahmad (1985). It is possible to match the displacement of the elastic dislocation to that of the simulation in order to determine an appropriate core-radius and core-energy. An attempt has been made to match the elastic field with atomic displacements calculated by Hansen (1994). The displacement fields match these atomic positions beyond about one burgers vector from the centre. The exact matching of the displacements has yet to be achieved, but preliminary work shows that a core radius of one burgers vector is not unrealistic. This is an unexpected result because, for semiconductors, Hooke’s law only holds for strains up to a few tenths of a percent, and with such a small core radius the strain at the edge of the core is approximately 10%.

In the absence of more useful results from atomic simulations it is necessary to make estimates of the energy stored in a core with a radius of one burger’s vector. Cottrell derived an expression for the energy by assuming that core experienced a strain equal to that found
at the core radius. This led him to calculate a core energy of $\approx 1.3 eV$/b which is independent of the core radius. Bragg (1947) and Huntingdon (1941) have also made estimates. Bragg assumed that the core energy density does not exceed the latent heat of fusion to obtain an estimate of $\approx eV$/b, and Huntingdon considered the electrostatic interaction between atoms to find $\approx 0.5 eV$/b.

From Ahmad (1985), the formation energy of a single vacancy for a pure silicon crystal is 2.776eV and for Germanium it is 2.433eV. A dislocation core, with $r_0 = b$, can be envisaged as many single vacancies added together in a line. Many of the dangling bonds which contribute to the energy will be able to link to bonds in the adjacent vacancies, and therefore the core energy density will be less than that of a single vacancy. An estimate of $1.5 eV$/b does not seem unreasonable.

5.6.3 Surface step energy

The 60° threading dislocation has a screw component, and a step is introduced at the surface of the cap as the threader glides. It is usual to assign an energy equal to the additional surface area that is introduced, multiplied by the surface energy density of the material. The additional area per unit length for a pure screw threader is equal to the Burger's vector, which means one dangling bond is added to the surface for each Burger's vector the threader glides. The energy of a dangling bond for Silicon or Germanium is roughly 1eV.

5.6.4 Surface relaxation

The cap is the last part of the structure to be grown; therefore, during growth the layers are uncapped. Growth occurs at temperatures in the range 300°C to 900°C depending on the materials and the use to which the layer will be put [Hull et al. (1988) and Patrat et al. (1990)]. The extremes of the temperature range are often employed in the study of growth. Commonly GaAs/InGaAs layers are grown at temperatures in the range 500°C to 600°C [Howard et al. (1992)]. At the high temperatures involved in growth, the dislocations are much more mobile and kinetic barriers blocking nucleation may be overcome more easily.
Therefore it is useful to know the equilibrium critical thickness for an uncapped layer.

There are two significant differences between analysis for an uncapped and a capped layer. Most importantly there is only one interface at which a gliding threader introduces dislocation line. Secondly, for an uncapped layer, the dislocation is close enough to the surface for there to be significant surface relaxation. The presence of only one dislocation in the numerical integration can be accounted for by including only one dislocation stress field, and in the analytic integration only one line tension needs to be included. However it is much more difficult to account for the surface relaxation. The problem can be dealt with approximately through the use of image dislocations, but analyses like that of Freund (1990) are required to treat it properly.

The critical thickness predicted for a uncapped layer, ignoring all energies associated with the dislocation except for the line tension, is about half that for a capped layer. Therefore, a capped layer which is below equilibrium critical thickness may once have been, during its growth, an uncapped layer exceeding critical thickness. If the relaxation occurs very quickly it is possible that the layer might relax completely before the cap is grown, and if the process is slow then maybe no significant relaxation will occur. Therefore, the investigation of uncapped layers, before the growth of a cap, requires study of the kinetics of the relaxation mechanisms.

5.6.5 Further elasticity-theory considerations

Semiconductors are anisotropic. The elastic theory used in this chapter assumes isotropy, therefore it is not a correct model for the strained layers. It is possible to carry out the same analysis incorporating the anisotropy, but the additional effort this requires is unlikely to produce significantly different results. If the stiffness of the material is very different in the direction of burgers vector which acts to relieve strain to that which does not, a different critical thickness may be predicted. However, it is more likely that anisotropy might result in one type of dislocation being slightly more energetically-favourable than another; thus influencing the character of the strain-relieving dislocation network.

The material in the strained layer is different to that in the cap and substrate, and the
Material | InP | GaAs | InAs | Si | Ge  
--- | --- | --- | --- | --- | ---  
C\textsubscript{11} | 102.2 | 118.8 | 83.3 | 165.8 | 128.5  
C\textsubscript{12} | 57.3 | 53.8 | 45.3 | 63.9 | 48.3  
C\textsubscript{44} | 44.2 | 59.4 | 39.6 | 79.6 | 66.8  
Anisotropy coefficient | 0.51 | 0.55 | 0.48 | 0.64 | 0.60  

Table 5.1: Elastic constants and the anisotropy coefficient for a selection of semiconductor materials taken from Fitzgerald (1993), Baker and Arzt (1994) and Prins and Dunstan (1990). The anisotropy coefficient is mentioned by Faux and Haigh (1990) and is equal to \( \frac{C_{11} - C_{12}}{2C_{44}} \). It is a measure of the degree of anisotropy of a material. For an isotrope it is equal to 1.

elastic constants of each are slightly different. A dislocation in one material is attracted to or repelled from an interface depending on whether the second material on the side of the interface away from the dislocation is less or more stiff than the first material. Therefore, there is an associated energy correction to make. The correction is likely to be small considering the similarity of the elastic constants given in table 5.1.

5.7 Comparison of the modified theory to experiment

5.7.1 Applying the energy corrections

The energy corrections of section 5.6.4 will be ignored because they apply only to uncapped layers, and the corrections of section 5.6.5 will not be considered because they are both difficult to quantify and are likely to have a small effect in any case. The remaining corrections deal with integration around the core, the core energy and the surface-step energy, and can be included as simple additions to the line tension, which gives for the 60° dislocation,

\[
\Delta E_{\text{line}} = \frac{\mu b^2}{4\pi} \frac{1 - \nu^2}{1 - \nu} \cos^2 60° \ln \left| \frac{h}{r_0} + 1 \right| - \frac{\mu (b \sin 60°)^2 (1 - 2\nu)}{16\pi (1 - \nu)^2} + \frac{1.5\text{eV}}{b} + \frac{1.0\text{eV}}{b} \quad (5.18)
\]

The second term, the integral about the core, only includes the edge component
of the Burgers vector because only this component results in tractions that act through the cylindrical surface of the core. The third and fourth terms depend on the type of strain-relieving dislocation being considered. The values used above are estimates for the 60° dislocation and must be redetermined when calculating critical thickness for other dislocation types. Using the line tension of equation 5.18 with \( r_0 \) set to one burgers vector, one obtains the following expression for critical thickness for a 60° dislocation:

\[
\frac{h_e}{b} = \frac{1}{\epsilon \cos \lambda} \left\{ \frac{1 - \nu^2}{4\pi(1 + \nu)} \ln \left[ \frac{h_e}{b} + 1 \right] - \frac{3}{4}(1 - 2\nu) + \frac{2eV(1 - \nu)}{\mu b^3(1 - \nu)} \right\} \quad (5.19)
\]

It is instructive to consider the energy contributed to the line tension by each term in equation 5.18. For a layer thickness of 100Å, and for dislocations in GaAs, with a burgers vector of 4.00Å, the first term is \( +1.8 \times 10^{-9} \text{Jm}^{-1} \), the second is \( -5.6 \times 10^{-11} \text{Jm}^{-1} \), the third is \( +0.6 \times 10^{-9} \text{Jm}^{-1} \) and the last is \( +0.4 \times 10^{-9} \text{Jm}^{-1} \). The comparison of these energies shows how important the corrections are in determining the actual value of critical thickness predicted.

### 5.7.2 Experimental results

The variety of different experimental techniques which have been used to study critical thickness is large. Many of the techniques have very different sensitivities to the onset of plastic relaxation, which often makes comparison between different experiments difficult; and the comparison to critical-thickness theories concerning only the first dislocation contributing to relaxation is even more difficult. The review articles by Fitzgerald (1991) and Jain and Hayes (1991) demonstrate how hard comparison can be. Fritz (1987) gives a good explanation of the difficulties in comparing theory to experiment by modifying the standard Matthews theory to predict the apparent critical thickness for experiments with a finite resolution in the lattice parameter.

In spite of the difficulties, a comparison between theory and experiment is given in figure 5.17.

There are several points to note in figure 5.17. When all the appropriate energy corrections, mentioned in section 5.6, are applied to both theories, the difference between
Figure 5.17: The original equilibrium theory and the modified theory are compared to data taken from the literature. The two graphs show the same data, but that on the left shows a smaller region enlarged for clarity. Constants appropriate to layers of InGaAs grown on GaAs were used for comparison to data on single capped layers obtained by Elman et al. (1989), Drigo et al. (1989) and Weng (1989). The dashed lines are the predictions for 60° mixed-dislocations and the solid lines correspond to pure misfit dislocations; the curves that bend back on themselves are those of the original equilibrium theory. Unfilled symbols represent layers which were unrelaxed and filled symbols represent layers which were relaxed. Squares are taken from Drigo et al., circles from Weng and diamonds from Elman et al.
the original and the modified theories in the range of technological interest is insignificant. Even though only a small amount of data, which is considered reliable, is plotted in the figure, there is disagreement between the different sources of data. Finally, most of the experimental data implies a critical-thickness higher than that predicted by theory, which corresponds to the insensitivity of the experiments to the first strain relieving dislocations.

5.8 Discussion

The main aim of the work presented in this chapter is to modify the Matthews theory so that it behaves in a realistic manner at high strains. This is achieved and, in so doing, the approximation in the earlier equilibrium theories is highlighted. Consequently, the work on arrays of dislocations by, for example, Willis et al. (1990, 1991a, 1991b), and certain theories considering the nucleation of dislocations by, for example, Beanland (1992) will benefit from including the correction.

No attempt is made to incorporate the core and surface step energies in a rigorously correct way. In order to do this one must move away from the simplicity of elasticity theory and consider the atomic nature of the dislocation structures. By comparing the results of elasticity theory to that of atomic scale simulations, the elasticity theory is shown to give good results as close as five angstroms to the centre of the core. However, even if the elasticity theory is correct so close to the core, it cannot give information concerning the energy contained within the core itself. Given the significant influence of this energy, discussed in section 5.7.1, the atomic scale simulation will be very useful.

Comparison to experiment of the equilibrium theories that consider only one dislocation is difficult because experiments are usually only sensitive to a larger dislocation density; therefore, equilibrium theories for arrays of dislocations are required. As a final comment, it is important to realise that study of kinetics and nucleation, like that of Dodson and Tsao (1987, 1988), of the strain-relieving dislocations may provide very important information concerning plastic relaxation, especially for capped layers below critical thickness which were once, during growth, uncapped layers above critical thickness.
Chapter 6

Discussion

Calculations of the strain distributions in a variety of structures and an extension to the equilibrium theory of critical thickness are presented in this thesis. The Fourier-method for calculating strain distributions in rectangular blocks is extended to include tangential stresses applied to the surfaces of the block. The extension to link several rectangular blocks in order to treat more complicated structures is discussed. A Green-function method for calculating the strain distributions about buried inclusions is presented. Chapter 5 presents a detailed discussion of the equilibrium theory of critical thickness and suggests some improvements which may be incorporated.

The Fourier-series method is also used to calculate the strain relaxation near the end facet of a strained-layer laser. In a compressive layer, the relaxation reduces the band gap near the facet and thus increases the optical absorption and, therefore, the relaxation might be a source of degradation of the facet. The calculated strain distribution is used as the basis for a calculation of the optical absorption. The results of the calculation showed that the absorption increases enough to cause degradation of the laser, and formed part of a patent application based on combining tensile and compressive layers in a way which inhibits relaxation.

The analysis of the end facet relaxation could be extended to include the relaxation occurring in the tensile barriers of a strain-compensated structure and, more importantly perhaps, to consider the effect for tensile layers. In a laser whose active region is a tensile
layer, the end facet relaxation will cause an increase in the band gap and so act to decrease optical absorption near the facet.

One of the aims of this thesis was to extend the Fourier-series method of Faux (1994) to treat linked blocks, in order to calculate strain distributions for strained over-layers and buried layers. The work presented in chapter 2 shows that, while this is in principle possible, the simplicity of the Fourier-series method for a single block is largely lost. However, the extension to include tangential forces as boundary conditions is useful and could profitably be used to analyse the strain relaxation of certain TEM samples more thoroughly.

In chapter 3 a Fourier-integral method is presented for calculating the stress distribution for an arbitrary force applied to the surface of a semi-infinite medium. The Fourier-integral method is used to calculate the stress field for a point force acting at the surface and it was shown that this could be used as a Green-function for calculating stress distributions for forces applied to surfaces. This idea could be extended, perhaps moving into the regime of boundary-element analysis, to include finite structures.

The Green-function method presented in chapter 4 provides a simple alternative to the Fourier-series method for calculating the strain fields about buried inclusions in an infinite medium. The strain field about a buried layer together with the simple analysis of the electronic properties shows that the band gap is constant over the cross-section of the layer but the degeneracy of the valence band is split by the axial strain in the buried layer. It would be useful to extend the analysis to inclusions that are not just rectangular in shape; for example, triangular and crescent-shaped quantum wires could be analysed. A more complete analysis of the effects of the strain relaxation on the electronic properties, incorporating more than just the zone-centre effects, would be useful. The occurrence of strain relaxation also means that piezoelectric effects might be observed for strained layers which if unrelaxed would not normally exhibit piezoelectricity.

The critical thickness theory presented in chapter 5 modifies the equilibrium theory in the literature, so that it is physically realistic at high strains. The reason that the previous result is incorrect at high strains is shown to an artefact of the integration for the energy of a dislocation. Future work could involve the incorporation of this modification in more
advanced critical thickness theories which deal with arrays of dislocations. Ultimately the equilibrium theories are limited to determining the thickness at which the presence of a strain-relieving dislocation is energetically favourable. Many experimental results indicate that the plastic relaxation of strained layers is not simply an equilibrium process and that the kinetics of the relaxation process are important.

A more useful way of studying the relaxation is, perhaps, through molecular dynamics. However, to date the vast computational requirement for dealing with the thousands of atoms that make up a very small section of a thin layer, limits such calculations; at most they can deal with only a single dislocation. It might be possible to model the relaxation by treating the dislocations themselves as the interacting objects. In this way the computational requirements could be significantly reduced, more than one dislocation could be studied and the interactions between dislocations might be modelled. The author envisages a model in which there are many different types of 'dislocation element', one corresponding to each of the dislocation types possible for the given crystal structure, which will be equal to the shortest possible segment of dislocation of that type.

In order to implement this 'dislocation dynamics' fully, it would be necessary to quantitively combine the atomic studies of the core structure with the elastic stress fields for many different dislocation and defect types. This procedure in itself would be very time consuming. Initially, a study of the motion of a single threader through a region of strained crystal would be appropriate and, perhaps later, the interaction between multiple dislocations might be modelled. Ultimately, nucleation mechanisms like the Hagan-Strunk, Frank-Read and spiral sources might be simulated.

By combining the strain distributions into a 'dislocation dynamics' simulation, which should also include more simple defects like the model of Hopgood (1994), it might be possible to model a complete device, perhaps even during operation. The author feels that, by combining models at different scales, it will be possible to produce a general model which will be useful to device designers and crystal growers.
## Indicial and Cartesian Notation

<table>
<thead>
<tr>
<th>Indicial</th>
<th>Cartesian</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1$</td>
<td>$x$</td>
<td>orthogonal coordinate</td>
</tr>
<tr>
<td>$x_2$</td>
<td>$y$</td>
<td>orthogonal coordinate</td>
</tr>
<tr>
<td>$x_3$</td>
<td>$z$</td>
<td>orthogonal coordinate</td>
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<tr>
<td>$u_1$</td>
<td>$u$</td>
<td>displacement in the $x$ direction</td>
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<tr>
<td>$u_2$</td>
<td>$v$</td>
<td>displacement in the $y$ direction</td>
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<tr>
<td>$u_3$</td>
<td>$w$</td>
<td>displacement in the $z$ direction</td>
</tr>
<tr>
<td>$\sigma_{11}$</td>
<td>$\sigma_{xx}$</td>
<td>stress acting normal on a surface perpendicular to the $x$ direction</td>
</tr>
<tr>
<td>$\sigma_{12}$</td>
<td>$\sigma_{xy}$</td>
<td>stress acting parallel to $y$ direction on a surface perpendicular to the $z$ direction</td>
</tr>
<tr>
<td>$\epsilon_{11}$</td>
<td>$\epsilon_{xx}$</td>
<td>$\frac{\partial u}{\partial z}$ or strain in $x$ direction</td>
</tr>
<tr>
<td>$\epsilon_{12}$</td>
<td>$\epsilon_{xy}$</td>
<td>$\frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial z} \right)$ or shear strain</td>
</tr>
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