Calculating Strain Using Atomistic Simulations: a Review

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Abstract. We present a short review of methods of evaluating of strain from atomistic models in the context of linear elasticity.

1. Introduction
The use of strain to tune semiconductor device performance has been an important area of research since 1970. It is well known that it is possible to grow a semiconductor overlayer on the top of a thick layer substrate even if the lattice constants of the two layers are different. A large strain can be then built into the overlayer, while still maintaining a long range atomic ordering in registry with the substrate monolayers. In the late 1940s Frank and Van der Merwe provided essential understanding of this pseudo-morphic growth in their classic papers and they proposed a theory of epitaxy where layer growth occurs with lattices relaxed by misfit on the substrate. According to experimental work, so long as the lattice mismatch is below roughly 10% it is possible to grow an epitaxial film which is in complete cohesion with the lattice substrate; the largest thickness achievable is called the critical thickness. Beyond the critical thickness there will be dislocations and as a result the atomic planes in the growth direction won’t accurately align.

Strain is the result of a relatively small displacement of the atoms in the crystal lattice. The strain affects the materials properties of the semiconductor, like e.g. the lattice constant, energy gap and effective masses of electrons and holes.

In the next sections we will review some of the basic concepts of elasticity in cubic crystals and further we will show how atomistic approaches can be used to extract the strain tensor directly from the atomic bonds.

2. Elasticity
For a cubic crystal it is possible to describe the strain (i.e. the ratio between the change as a result of stress and its original state) in the system by imaging a set of orthonormal vectors $\hat{x}$, $\hat{y}$, $\hat{z}$ in the unstrained system. As a result of the influence of a uniform deformation the axes will be distorted to $x'$, $y'$, $z'$. The new axes can be related to the previous ones by:

$$x' = (1 + \varepsilon_{xx}) \hat{x} + \varepsilon_{xy} \hat{y} + \varepsilon_{xz} \hat{z}$$
$$y' = \varepsilon_{yx} \hat{x} + (1 + \varepsilon_{yy}) \hat{y} + \varepsilon_{yz} \hat{z}$$
$$z' = \varepsilon_{zx} \hat{x} + \varepsilon_{zy} \hat{y} + (1 + \varepsilon_{zz}) \hat{z}$$

(1)
The deformation in the system is defined by the coefficients $\varepsilon_{\alpha\beta}$. The new axes which have been created are not orthogonal in general. At the point $r$ the effect of the deformation in the unstrained coordinates is:

$$\mathbf{r} = x\hat{x} + y\hat{y} + z\hat{z}$$

(2)

Then the new vector after distortion is:

$$\mathbf{r}' = x\hat{x}' + y\hat{y}' + z\hat{z}'$$

(3)

Note that the coefficients $x, y, z$ are unchanged while the new strained basis vectors are no longer necessarily unitary. The displacement caused by the deformation can be found from:

$$\mathbf{R} = \mathbf{r}' - \mathbf{r} = x(\hat{x}' - \hat{x}) + y(\hat{y}' - \hat{y}) + z(\hat{z}' - \hat{z})$$

$$\mathbf{R} = (x\varepsilon_{xx} + y\varepsilon_{yx} + z\varepsilon_{zz})\hat{x} + (x\varepsilon_{xy} + y\varepsilon_{yy} + z\varepsilon_{zy})\hat{y} + (x\varepsilon_{xz} + y\varepsilon_{yz} + z\varepsilon_{zz})\hat{z}$$

(4)

This can be written by defining the quantities $u, v, w$:

$$\hat{R}(r) = u(r)\hat{x} + v(r)\hat{y} + w(r)\hat{z}$$

(5)

In the small strain limit:

$$x\varepsilon_{xx} = x\frac{\partial u}{\partial x}; y\varepsilon_{yy} = y\frac{\partial v}{\partial y}; z\varepsilon_{zz} = z\frac{\partial w}{\partial z}$$

(6)

Instead of using the 9 distortion components $\varepsilon_{ij}$ to describe deformation, the strain components $e_{ij}$ are conventionally used, defined by:

$$e_{xx} = \varepsilon_{xx} = \frac{\partial u}{\partial x}; e_{yy} = \varepsilon_{yy} = \frac{\partial v}{\partial y}; e_{zz} = \varepsilon_{zz} = \frac{\partial w}{\partial z}$$

(7)

The off-diagonal terms describe the angular distortion due to strain and can be written as:

$$e_{xy} = \varepsilon_{xy} = \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}$$

$$e_{yz} = \varepsilon_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}$$

$$e_{zx} = \varepsilon_{zx} = \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}$$

(8)

It is worth noting how there is often confusion about the difference between strain and distortion components. In general there are 9 independent distortion components but only 6 strain components. However it is possible to find a basis transformation where the distortion matrix becomes triangular (upper or lower). In that case the non-zero distortions are exactly equal to the corresponding strain components.

The diagonal components of the strain or distortion tensor are those responsible for compressive or tensile strain. All the other components instead generate shear pressure. Conventionally technologists don’t need to deal with the full complexity of the strain tensor. In fact two dimensional epitaxial growth usually introduces only two strains, one parallel to the growth plane and one orthogonal (perpendicular strain). This happens because crystals tend to roughly conserve their volume and hence a negative (positive) pressure in the growth plane results in a counteracting positive (negative) pressure in the direction perpendicular to the plane.

It is often possible to estimate such strains easily using elastic theory, provided the elastic constants of the crystal are known. We are not going to formally define the elastic constants here. A formal derivation involving the stress-strain relations can be found in textbooks.

There are in general 36 elastic constants for a cubic crystal, but these can be reduced in real structures by utilizing symmetry arguments. For zinc-blende such symmetries reduce the total number to only...
3 independent constants: \(c_{11}, c_{12}, \text{ and } c_{44}\). In a wurtzite crystal instead symmetry is lower and hence there are 5 independent elastic constants: \(c_{11}, c_{12}, c_{13}, c_{33}, \text{ and } c_{44}\).

In the zinc-blende crystal the 3 elastic constants are linked to particular deformations that in practice are difficult to achieve independently from each other. Deformations that are more practical are those described by the Bulk Modulus \((B)\) and Shear constant \((C')\). For a zinc-blende crystal, \(B\) and \(C'\) are given by:

\[
B = \frac{1}{3} (c_{11} + 2c_{12})
\]

\[
C' = \frac{1}{2} (c_{11} - c_{12})
\]

However both the Bulk modulus and Shear constant can be easily expressed in terms of the second derivatives of the total energy of the system,

\[
B = \frac{1}{\Omega} \left. \frac{d^2 E}{d\nu^2} \right|_{E=E_{\text{tot}}}
\]

\[
C' = \frac{1}{\Omega} \left. \frac{d^2 E}{d\varepsilon^2} \right|_{E=E_{\text{tot}}}
\]

Where \(\Omega\) is the atomic volume which for zinc-blende or diamond is equal to \(a^3/8\) (\(a\) is the lattice constant). The expressions in Eqs. 11 and 12 provide a link to evaluating \(B\) and \(C'\) from interatomic potentials that give the total energy \(E\). For the Bulk Modulus, \(\nu\) expresses the uniform deformation (hydrostatic) of any vector \(R'\) in the crystal:

\[
R' = \nu^\frac{1}{3} R
\]

While the shear constant \(C'\) is defined through the non-uniform deformation:

\[
R'_x = R_x (1 + \varepsilon) \\
R'_y = R_y (1 + \varepsilon) \\
R'_z = R_z
\]

Such strains are realistic and provide a meaningful way of relating 2 of the 3 elastic constants to practical deformations. However it is worth noting how these deformations so far only modify the lattice vectors length and not the angle between them.

The third elastic constant \(c_{44}\) is instead related to the deformations which alter the angles between the lattice vectors:

\[
R'_x = R_x + \gamma R_y \\
R'_y = R_y \\
R'_z = R_z
\]

So that the relevant second derivative of the total energy is:
This evaluation is not straightforward. When performing the calculation one needs to take into account the internal displacements which move the interpenetrating fcc sublattices in the diamond structure along the z axis, and hence minimise the energy for every given \( \gamma \), with respect of this internal displacement. This distortion has a deep meaning. In fact in a single tetrahedron with one atom in the centre of the coordinate system, a positive shear distortion would pull apart the two atoms along the [110] direction, while simultaneously pushing closer the other two atoms in the [\(1 \bar{1} 0\)] direction. As a result of these movements the atom at the centre of the tetrahedron is under radial and angular forces, which resist changes to bond lengths and bond angles respectively. The displacement that minimises the total energy (typically a downwards shift orthogonal to the shear plane for a positive shear) is a consequence of a subtle balance among the two forces and results in different bond lengths within the same tetrahedron.

This elastic behaviour has an important and often overlooked consequence: the 6 components of the strain tensor alone cannot define all possible strain states of a crystal. For shear strains a further quantity must be known to define the amount of internal displacement. Such quantity is well known and usually referred to as Kleinman’s internal displacement parameter \( \zeta \), which defines the distance among the two sublattices as being \( \zeta \gamma / 4 \) of the lattice constant \( a \).

For the wurtzite structure similar definitions exist for the Bulk Modulus, Shear constant and Kleinman parameter which can be found in the literature.

### 3. Evaluating Strain from an Atomistic Structure

Strain is usually a concept better suited to describing deformations in cubic cells and often one thinks of the entire crystal being composed by a series of cubic unit cell blocks. However strain also clearly affects the atomic positions within those blocks. Here we try to merge the two pictures and explain how to extract the strain tensor from atomic positions. This is useful in order to extract information from the result of e.g. Molecular Dynamics (MD). From Figure 1 we notice that each atom of a strained or unstrained crystal is always inside a tetrahedron. Hence by comparing each tetrahedron in a strained structure with a chemically equivalent bulk tetrahedron one can relate strained and unstrained lattice vectors and derive the components of the strain tensor.

Irrespective of the crystal structure, provided the x, y and z are chosen so that the [111] direction for zinc-blende corresponds to the [0001] for wurtzite, such comparison results in a simple system of 6 linear equations to finally obtain the components of the deformation tensor and hence the strain tensor. In practice this is done in the following way: there are 4 vectors connecting the second nearest neighbours surrounding the atom inside the tetrahedron. As there are only three degrees of freedom, one can in principle chose any three out of the four vectors. Whatever the particular choice of vectors, the problem becomes that of solving the three matrix problems of the form:

\[
\begin{pmatrix}
1 + \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & 1 + \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & 1 + \varepsilon_{zz}
\end{pmatrix}
\begin{pmatrix}
 a \cdot x_i \\
 a \cdot y_i \\
 a \cdot z_i
\end{pmatrix}
= \begin{pmatrix}
 a \cdot x_i' \\
 a \cdot y_i' \\
 a \cdot z_i'
\end{pmatrix}
\]

\[i = 1, 2, 3\]
following the notation with and without the superscript to indicate strained and unstrained Cartesian coordinates and reminding that \( a \) is the lattice constant of the bulk material. Once solved the components of the distortion tensor can be easily related to those of the elastic strain by reminding that \( e_{ij} = e_{ij} \) and that:

\[
\begin{align*}
\varepsilon_{xy} &= \vec{x}' \cdot \vec{y}' = \varepsilon_{xy} (1 + e_{xx}) + \varepsilon_{yx} (1 + e_{yy}) + e_{xz} \cdot e_{yz} \\
\varepsilon_{xz} &= \vec{x}' \cdot \vec{z}' = \varepsilon_{xz} (1 + e_{xx}) + e_{zx} (1 + e_{yy}) + e_{xy} \cdot e_{yz} \\
\varepsilon_{yz} &= \vec{y}' \cdot \vec{z}' = \varepsilon_{yz} (1 + e_{yy}) + e_{zy} (1 + e_{xx}) + e_{xy} \cdot e_{zx}
\end{align*}
\]

The last expression is calculated without assuming the small strain limit as in Eq. 8. The difference is often small but since these operations are usually automatically computed there is no need to introduce any approximations.

![Figure 1: The unstrained and strained tetrahedron.](image)

As explained earlier these set of operations fulfill the task of obtaining the 6 components of the strain tensor but does not provide any information on the sublattice displacement. In fact the position of the atom inside the tetrahedron does not enter the calculation at all. This is because the sublattice displacement can only be determined after the strain components have been identified. To identify the sublattice displacement one needs to first of all determine the ideal position (after strain but before any displacement) of the central atom within the tetrahedron. Then upon comparing the actual position and the ideal position (as calculated by simply applying the deformation tensor to the unstrained case, without considering internal relaxation) one obtains the displacement \( \delta r \). Such displacement can then be related to the Kleinman\(^4\) parameter, which for convenience should be expressed as a 3D vector:

\[
\begin{align*}
\delta x &= \frac{a \cdot \zeta_x \cdot e_{xx}}{4 (1 + e_{xx})} \\
\delta y &= \frac{a \cdot \zeta_y \cdot e_{yy}}{4 (1 + e_{yy})} \\
\delta z &= \frac{a \cdot \zeta_z \cdot e_{zz}}{4 (1 + e_{zz})}
\end{align*}
\]

The reason to express the Kleinman\(^4\) parameter as a vector is that recent work suggested that there is a strong dependence on strain for this quantity and hence even the word parameter is misleading.\(^7,8,9\)

### 4. Alloys

The method outlined in the previous section is general and applicable to both pure and alloyed semiconductors. In both cases however one needs to clarify what the reference point is. In fact there
are two ways of defining strain. The first, often used by experimentalists, particularly electron microscopists, is to relate the increased or decreased lattice spacing of the particular semiconductor material or alloy one is studying in respect of that of the substrate or matrix material. This is obviously useful to experimentalists since the background material provides the calibration for the measurement. Alternatively, as theorists tend to do instead, the strain status is thought to be the deformation from the unstrained bulk case of the same material. The strain in this case is directly the quantity that is needed as input to evaluate the bandstructure modifications through strain.

The former presents however an inherent difficulty. For a semiconductor alloy the reference lattice parameter needs to be that of its theoretical unstrained case, which is often evaluated from Vegard’s law as an interpolation between binary compounds, for a given composition. However such composition in some cases (e.g. diffused or graded interfaces) is a local property of the alloy. Since it is difficult to evaluate such local composition from the first nearest neighbours alone, it is generally suggested to choose a suitable sphere around one atom and to obtain the composition by atom counting over several rings of nearest neighbours. This will give a suitable estimate of the local composition.

5. Practical Aspects of Evaluating Strain

In order to evaluate the strain tensor of a system of atoms whose positions are determined by MD, the following sequence of steps is required for each atom $i$:

1) Determine the 4 nearest neighbours. This is sometimes part of the MD output, but if not then it can be easily evaluated by searching through the atoms list within a small radius (dependent on the lattice parameter of the material) of the atom $i$. This is a triangular problem (if $i$ is a neighbour of another atom $j$, then the opposite is also true) hence the search can be implemented rather quickly by avoiding searching twice on the same atoms.

2) Determine the local composition, as described in section 4, and use it to evaluate the local unstrained bond length, in the framework of Vegard’s law (using also the local composition) in the case of alloys.

3) Use the nearest neighbour list obtained during the first step to identify the coordinates of the nearest neighbours and use together with the local unstrained bond length obtained during step 2 in conjunction with Eqs. 17-18. Solve the resulting set of equations to obtain the 6 components of the strain tensor.

4) With the distortion components determined during step 3, determine the ideal position of atom $i$ in respect of the four nearest neighbours by applying the distortion tensor to an unstrained set of atoms belonging to a material where the composition and lattice constant are those obtained during step 2. The difference between the ideal position and that found from the MD output gives $\delta x$, $\delta y$ and $\delta z$ of Eq. 19, from which the Kleinman parameter is readily obtained. This step is normally not needed in most cases. We have previously noted how it is an important quantity if a comprehensive atomistic description of piezoelectricity is required.

We will now show a sample of such strain calculations for a series of rather complicated structures consisting of a GaAs substrate, a thin two dimensional InAs layer, a three dimensional quantum dot island, a capping formed by a non uniform InGaAsSb alloy (with different Sb content for the 3 models) and a further GaAs capping.

We will only show the diagonal components of the strain, though the full strain tensor was calculated, as the diagonal components are those that contain more information about the lattice deformation.
What is noticeable from figure 2 is that by using atomistically determined strain maps it is possible to obtain smooth strain profiles in the regions where only binary semiconductor compounds are present. In the alloyed regions instead compositional disorder plays an important role and strain maps reproduce the coarse nature of the underlying material. In that respect this shows how, by preserving the nature of the material under study, atomistic modelling produces more realistic results compared to e.g. continuum elasticity theory.

6. Conclusions
So far we have described the mathematic involved in the evaluation of the strain from a relaxed atomistic model. Describing the force fields (e.g. bond order potentials\textsuperscript{12}, Keating’s Valence Force Field\textsuperscript{13} and Stillinger-Weber potential\textsuperscript{14} that can be used to obtain the relaxed geometry is beyond the scope of this short review. The methodology that we presented is general and can be used effectively and accurately in most atomistic level modelling of strain properties of semiconductor crystals.

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