

Non-linear strain theory for low-dimensional semiconductor structures

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Abstract

We present a continuous non-linear strain theory and demonstrate its plausibility on modelling low-dimensional semiconductor nanostructures. The main advantages of this theory are its non-linearity, continuous nature (computationally inexpensive), and anisotropy (includes the crystal structure). The theory allows us to account explicitly for internal strain and for realistic interface boundary conditions. The discussion is restricted to cases where the strain is nearly constant on the length scale of the primitive lattice cell except at interfaces where discontinuities are allowed. The main idea behind the theory presented here is to include as much information on the atomic structure in the continuous limit as it is necessary in order to accurately describe nanoscale systems. To illustrate the importance of non-linear effects and the inclusion of internal strain, we present some simple calculation for quantum wells with diamond crystal structure oriented in the $[1\ 1\ 1]$ direction.

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1. Introduction

Many nanoscale semiconductor heterostructures of experimental and theoretical interest consist of materials with a lattice mismatch of up to 13%, for example, InAs/GaAs and Sn/Ge [10]. This lattice mismatch is the driving mechanism for one of the fabrication methods used to construct nanoscale devices (self-assembly). In addition, it is known that strain

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strongly affects the electronic and optical properties of nanoscale structures. This fact has important implications and, among other things, has allowed to construct better quantum well lasers [3]. Strain contributions are essential in a realistic description of most self-assembled nanostructures. Until now, strain calculations for such structures have mainly been based on either an atomistic model (Valence Force Field) [8] or one of the continuous linear strain models (e.g., [2,5,9]). While atomistic models are computationally expensive making them difficult to apply to many important low-dimensional semiconductor structures (LDSS), the conventional continuous models applied to modelling of LDSS do not include non-linear effects and internal strain explicitly nor do they employ the correct interface boundary conditions. Internal strain refers to internal displacements of sublattices not determined by symmetry alone [4]. In this contribution, we present a continuous non-linear theory for modelling LDSS and discuss its applications in the context of modelling diamond quantum well nanostructures. We compare results obtained with known linear models and those obtained on the basis of the non-linear theory.

2. Theory

In this section, we present the theory behind the non-linear strain model we propose to use for LDSS strain calculation. We start with a description of the strain theory in the atomistic framework for bulk materials. This is followed by an explanation of how such a description can be taken to the continuous limit, i.e., how to define continuous quantities that capture the physics of the problem. And finally, we show how to extend the presented theory to heterostructures.

2.1. Atomistic picture—bulk material

The atomistic picture of crystalline materials is based on a semi-classical description of these structures, i.e., atoms are treated as point particles arranged in a periodic lattice. This periodic structure is best described by the primitive lattice cell and a set of vectors w_j , where $j = 1, \dots, j_{\max}$, giving the position of the atoms inside the primitive lattice cell. The primitive lattice cell is the smallest repeated parallelepiped making up the crystal structure. Letting v_1 , v_2 and v_3 denote the three edge vectors of the primitive lattice cell, we find that a given atomic position a_{ij} (the j th atom in the i th primitive lattice cell) can be expressed as follows:

$$a_{ij} = \sum_{q=1}^3 c_q v_q + w_j, \quad (1)$$

where $c_q \in \mathbb{Z}$.

For strain energy calculations, it is not the actual position of the atoms that matters but rather the vectors connecting the different atoms. These vectors are called position vectors and they are given as follows:

$$X_{kj}(a_{ij}) = a_{ip} - a_{ij}, \quad (2)$$

i.e., the vector with a_{ij} as base point and a_{lp} as end point. The reason why we do not include indices l and p on the left-hand side is that we need the following property later on: the index k is used to label the position vectors such that

$$X_{kj}(a_{ij}) = X_{kj}(a_{i'j}) \quad (3)$$

for all $i, i' \in \{1, \dots, i_{\max}\}$ and $j \in \{1, \dots, j_{\max}\}$, where i_{\max} is the number of primitive lattice cells. This is possible because we have a periodic structure.

In principle, we should account for all the position vectors when we calculate the strain energy, but because the forces between atoms are short ranged we only need to take into account a small subset. We label these such that $k = 1, \dots, k_{\max}$. Usually, the position vectors of the nearest or second nearest neighbors are enough to capture the physics of the problem.

The total energy before any deformation is now given by

$$V_0 = \frac{1}{2} \sum_{i=1}^{i_{\max}} \sum_{j=1}^{j_{\max}} V_j(\langle X_{kj}(a_{ij}), X_{pj}(a_{ij}) \rangle), \quad (4)$$

where V_j is the energy contribution from the j th atom in the primitive lattice cell. It is a function of the standard inner product in \mathbb{R}^3 between all possible combinations of the position vectors with the specified atom as origin, i.e., all possible combinations of k and p .

A deformation of the crystal is given by an injective map $\phi_{\text{mic}}: A \rightarrow \mathbb{R}^3$, where A is the set of initial atomic positions and the position vectors are transformed according to

$$\Phi(X_{kj})(\phi_{\text{mic}}(a_{ij})) = \phi_{\text{mic}}(a_{lp}) - \phi_{\text{mic}}(a_{ij}), \quad (5)$$

this is just the position vectors of the deformed crystal. As long as we do not include all position vectors in our model we cannot treat all possible deformations. This is because a deformation can bring atoms, that before the deformation had a negligible influence on the energy (the position vector between them was not included in the energy), close enough together such that the contribution cannot be neglected anymore. The rule is that we need to include as many position vectors as is necessary to describe the kind of deformations we are interested in.

The strain energy is then given by the total energy of the deformed crystal minus the total energy of the undeformed crystal, i.e.,

$$V(\phi_{\text{mic}}) = \frac{1}{2} \sum_{i=1}^{i_{\max}} \sum_{j=1}^{j_{\max}} V_j(\langle \Phi(X_{kj})(\phi_{\text{mic}}(a_{ij})), \Phi(X_{pj})(\phi_{\text{mic}}(a_{ij})) \rangle) - V_0. \quad (6)$$

Making a second-order Taylor expansion of this produces the well-known Valence Force Field model [7].

2.2. Continuum limit

In order to pass to the continuum limit, we have to define some continuous quantities that capture the important physics of the problem. First, we specify extensional characteristics of the material:

Definition 2.1 (*Crystal volume*). The crystal volume \mathcal{B} is defined to be the union of all the primitive lattice cells making up the material.

This definition may not be appropriate if one wants to describe surface effects, because the surface of the crystal volume defined in this way is too irregular. But we are not interested in surface effects, hence Definition 2.1 is a reasonable definition of the crystal volume.

The next quantity we need to define in the context of the continuum limit is the position vectors. We saw in the last section (Eq. (3)) that the position vectors with one atom as base point is identical to the position vectors with another atom of the same kind (the same j index) as base point (just parallelly translated to the other atom). This suggests the following definition.

Definition 2.2 (*Position vector fields*). The position vector fields X_{kj} are defined to be the constant vector fields, $X_{kj}(\vec{r}) = X_{kj}(a_{ij})$ for all $\vec{r} \in \mathcal{B}$.

With the help of these two definitions it is easy to show that the total energy before a deformation (Eq. (4)) is given by

$$V_0 = \frac{1}{2} \sum_{j=1}^{j_{\max}} \int_{\mathcal{B}} \frac{V_j(\langle X_{kj}(\vec{r}), X_{pj}(\vec{r}) \rangle)}{V_p} d\vec{r}^3, \quad (7)$$

where V_p is the volume of the primitive lattice cell. It should be noted here that we have made no approximations going from Eqs. (4) to (7).

We need a rather complex definition of deformations. This is because we want to average out the behavior on the scale of the primitive lattice cell, but still ensure that we do not lose any physical important behavior. This is done by explicitly including the behavior of the w_j vectors.

Definition 2.3 (*Deformation*). Let E be the set of constant vector fields on \mathcal{B} given by the w_j vectors. A map $\phi: E \rightarrow T\mathbb{R}^3$, where $T\mathbb{R}^3$ is the tangent bundle over \mathbb{R}^3 , is a deformation compatible with the atomistic deformation ϕ_{mic} if and only if

$$\pi_{\mathbb{R}^3} \circ \tilde{\phi}(w_j) = \pi_{\mathbb{R}^3} \circ \tilde{\phi}(w_{j'}) \quad \text{for all } j, j' = 1, \dots, j_{\max} \quad (8)$$

and

$$\phi(a_{i0}) + \tilde{\phi}(w_j)(\phi(a_{i0})) = \phi_{\text{mic}}(a_{ij}) \quad \text{for all } a_{ij}, \quad (9)$$

where $\phi = \pi_{\mathbb{R}^3} \circ \tilde{\phi} \circ \pi_{0,\mathcal{B}}^{-1}$,

$$\begin{array}{ccccc} & & \tilde{\phi} & & \\ & & \downarrow & & \\ \pi_{0,\mathcal{B}} & w_0 & \rightarrow & T\mathbb{R}^3 & \\ & \updownarrow & & \downarrow & \pi_{\mathbb{R}^3} \\ & \mathcal{B} & \rightarrow & \mathbb{R}^3 & \\ & & \phi & & \end{array}$$

and $\pi_{0,\mathcal{B}}$ and $\pi_{\mathbb{R}^3}$ are the projection maps onto \mathcal{B} and \mathbb{R}^3 , respectively.

The idea is that ϕ captures the macroscopic behavior and $\tilde{\phi}$ captures the microscopic behavior (inside the primitive lattice cell).

In order to find a good approximation of the transformation of the position vector fields X_{kj} in the continuous framework, we need the observation that

$$X_{kj}(a_{ij}) = w_l - w_j + \sum_{q=1}^3 d_q v_q \quad (10)$$

for some $d_q \in \mathbb{Z}$, where w_l is the vector giving the position of the atom inside the primitive lattice cell that $X_{kj}(a_{ij})$ points to. The term involving the sum is just the vector with base point in the primitive lattice cell that includes a_{ij} and end point in the primitive lattice cell that includes the atom that $X_{kj}(a_{ij})$ points to. We now have

Theorem 2.1. *The transformation of the position vectors $X_{kj}(a_{ij})$ is to the first order in ϕ given by*

$$\Phi(X_{kj})(\phi_{\text{mic}}(a_{ij})) \approx \phi_{\star} X_{kj}(\phi_{\text{mic}}(a_{ij})) + u_l(\phi_{\text{mic}}(a_{ij})) - u_j(\phi_{\text{mic}}(a_{ij})), \quad (11)$$

where $\phi_{\star}: T\mathcal{B} \rightarrow T\mathbb{R}^3$ is the push-forward operator on vector fields and $u_j = \tilde{\phi}(w_j) - \phi_{\star} w_j$ (known as internal strain [4,7]).

Proof. This is easily seen by making a first-order Taylor expansion of ϕ . \square

The operator ϕ_{\star} is in elasticity also known as the deformation gradient. This suggests that we should define the transformation of the position vector fields as follows.

Definition 2.4 (Transformation of the position vector fields). The transformation Φ of the position vector fields is given by

$$\Phi(X_{kj}) = \phi_{\star} X_{kj} + u_l - u_j. \quad (12)$$

It is now straightforward to show that, under the assumption that the transformation Φ is nearly constant on the length scale of the primitive lattice cell, the strain energy is approximately given by

$$V \approx \frac{1}{2} \sum_{j=1}^{j_{\max}} \int_{\mathcal{B}} \frac{V_j(\langle \Phi(X_{kj}), \Phi(X_{pj}) \rangle)}{V_p} \mathrm{d}r^3 - V_0. \quad (13)$$

In relation to other strain models it should be noticed that a second-order Taylor expansion of V and some approximation of the internal strain and the strain $\varepsilon = \frac{1}{2}(\phi_{\star}^T \phi_{\star} - I)$, where $I: T\mathcal{B} \rightarrow T\mathcal{B}$ is the identity map, produces the continuum linear mechanical model that has been used extensively in the context of LDSS modelling (e.g., [6]).

2.2.1. Diamond

As an example, we derive the total strain energy for materials with diamond crystal structure. The primitive lattice cell is in this case given by

$$v_1 = 2a[1, 1, 0], \quad v_2 = 2a[1, 0, 1], \quad v_3 = 2a[0, 1, 1],$$

where a is the lattice constant. There are two atoms inside the primitive lattice cell:

$$w_0 = [0, 0, 0], \quad w_1 = a[1, 1, 1]$$

and the nearest-neighbor position vectors are given by

$$X_1 = X_{10} = -X_{11} = w_1, \quad X_2 = X_{20} = -X_{21} = w_1 - v_1,$$

$$X_3 = X_{30} = -X_{31} = w_1 - v_2, \quad X_4 = X_{40} = -X_{41} = w_1 - v_3.$$

We see that the position vectors around the first atom in the primitive lattice cell are given by the negative of the position vectors around the second atom.

In order to get an expression that we can calculate we make a second-order Taylor expansion of V and assume that only the diagonal products of the inner product contribute to the strain energy, arriving at

$$V \approx \int_{\mathcal{B}} \left[\frac{\alpha}{4V_p} \sum_{i=1}^4 (\langle \phi_{\star}(X_i) + u_1, \phi_{\star}(X_i) + u_1 \rangle - \langle X_i, X_i \rangle)^2 + \frac{\beta}{2V_p} \sum_{i,j>i}^4 (\langle \phi_{\star}(X_i) + u_1, \phi_{\star}(X_j) + u_1 \rangle - \langle X_i, X_j \rangle)^2 \right] dr^3, \quad (14)$$

where α and β are fitting parameters.

2.3. Heterostructure

We are now in a position to consider the kind of heterostructures we are interested in. Namely, structures where one material is embedded in another material (see Fig. 1). We assume that the two materials have the same crystal structure but they are allowed to have different lattice constants. The first thing we need to do in order to find the strain energy is to define a reference configuration. We do this by shrinking or expanding the inner material by a homogeneous deformation such that the two materials have the same crystal structure and lattice constant (and the same orientation). Next, we split the structure into two regions. This is done according to the following rules:

- Ω_i contains all the atoms of material i ,
- all the primitive lattice cells are included in $\Omega_1 \cup \Omega_2$ and nothing else,
- the interface Γ between Ω_1 and Ω_2 consists of finitely many plane surfaces.

We note that the above procedure may not define the interface in a unique fashion, but further discussion of this issue falls outside of the scope of the present paper.

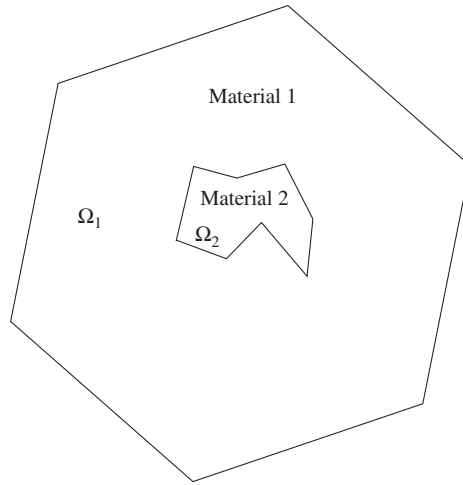


Fig. 1. System under investigation.

We are now able to find the strain energy of the whole system in three steps. First, we find the strain energy of material one

$$V_1 \approx \frac{1}{2} \sum_j \int_{\Omega_1} \frac{V_{1,j}(\langle \Phi(X_{kj}), \Phi(X_{pj}) \rangle)}{V_{p1}} dr^3 - V_{1,0}, \quad (15)$$

then we find the strain energy of material two

$$V_2 \approx \frac{1}{2} \sum_j \int_{\Omega_2} \frac{V_{2,j}(\langle \Phi(X_{kj}), \Phi(X_{pj}) \rangle)}{V_{p2}} dr^3 - V_{2,0}. \quad (16)$$

The last step is to find the strain energy resulting from the presence of the interface. This is done by projecting the additional contribution around the interface into the interface surface in the following manner.

Due to periodicity of the structure, the intersections of the position vectors with one specific plane surface will also be arranged in a periodic fashion. We can, as a consequence, describe the periodic structure on the interface by a 2-dimensional principal lattice cell and a set of 2-dimensional vectors \hat{w}_l giving the position of the intersections inside the primitive lattice cell. We denote with d_{nl} the l th intersection inside the n th primitive lattice cell and with $Z_{sl}(d_{nl})$ the vectors that intersect the surface at d_{nl} , where the index s is chosen such that

$$Z_{sl}(d_{nl}) = Z_{sl}(d_{n'l}) \quad (17)$$

for all $s = 1, \dots, s_{l,\max}$, $l = 1, \dots, l_{\max}$ and $n, n' = 1, \dots, n_{\max}$, where n_{\max} is the number of 2-dimensional primitive lattice cells, l_{\max} is the number of intersections inside the primitive lattice cell and $s_{l,\max}$ is the number of position vectors intersecting the surface at the l th intersection inside the primitive lattice cell. This is similar to what we did for the

3-dimensional crystal structure. In addition to this we denote by $\hat{X}_{tl}(d_{nl})$ all the position vectors of the atom that has $Z_{sl}(d_{nl})$ as origin. Again we have that

$$\hat{X}_{tl}(d_{nl}) = \hat{X}_{tl}(d_{n'l}) \quad (18)$$

for all $t = 1, \dots, t_{l,\max}$, $l = 1, \dots, l_{\max}$ and $n, n' = 1, \dots, n_{\max}$, where $t_{l,\max}$ is the number of position vectors around the atom that has $Z_{sl}(d_{nl})$ as origin. In order to get a structure that lives on the interface surface we parallelly translate $Z_{sl}(d_{nl})$ and $\hat{X}_{tl}(d_{nl})$ in such a way that they have d_{nl} as origin. If we now write down the contribution of the interface to the strain energy and take this to the continuum limit in the same manner as before, we arrive at

$$V_{\text{int}} \approx \frac{1}{2} \int_{\Gamma} \sum_{l=1}^{l_{r,\max}} \sum_{m=1}^2 \frac{V_{\text{int},l,m}(\langle \Phi_m Z_{sl}(\phi(\vec{r})), \Phi_m X_{tl}(\phi(\vec{r})) \rangle)}{A_p(\vec{r})} dA - V_{\text{int},0}, \quad (19)$$

where $A_p(\vec{r})$ is the area of the 2-dimensional interface primitive lattice cell (it is piecewise constant), $l_{r,\max}$ is the number of intersections inside the 2-dimensional primitive lattice cell (it is also piecewise constant) and the subscript m on Φ signifies that it is the limit of the functions taken from material m . The interface contribution $V_{\text{int},l,m}$ is a function of the inner product between all possible combinations of s and t .

The strain energy of the system is now given by

$$V = V_1 + V_2 + V_{\text{int}}. \quad (20)$$

It is minima of the strain energy of the system with respect to ϕ and u_j that give equilibrium strain tensors according to (there might be more than one minimum)

$$\varepsilon = \frac{1}{2}(\phi_{\star}^T \phi_{\star} - I). \quad (21)$$

3. Quantum well results

In this section, we present results of an implementation of the above optimization problem for a quantum well, i.e., a thin plate with a barrier material on both sides (see Fig. 2). The system is allowed to be deformed only in the direction of the well (perpendicular to the plate). We have chosen to investigate two material systems, Silicon in Germanium and Tin in Germanium, both with a diamond crystal structure.

The model has the following non-linearities: it is

- non-linear in the definition of the strain

$$\varepsilon = \frac{1}{2}(\phi_{\star}^T \phi_{\star} - I) = \frac{1}{2}(d_{\star}^T + d_{\star} + d_{\star}^T d_{\star}), \quad (22)$$

where $d = \phi - Id$ and $Id: \mathcal{B} \rightarrow \mathbb{R}^3$ is given by $Id(\vec{r}) = \vec{r}$, and

- non-linear with respect to the internal strain u_1 . Notice that u_1 is the only internal strain variable present in Eq. (14).

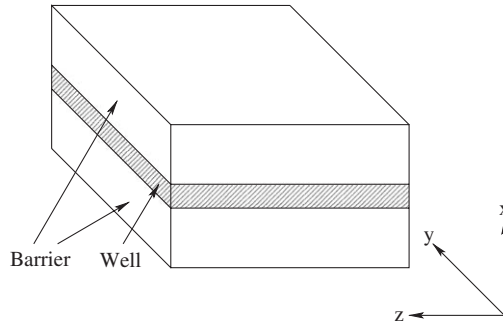


Fig. 2. The structure of a quantum well.

Because of that we have chosen to compare three different models.

- Model 1 (Non-linear):

This is the model we described in the previous section.

- Model 2 (Linear in u_1):

The $\langle u_1, u_1 \rangle$ terms are neglected in Eq. (14). This ensures that $\partial V / \partial u_1 = 0$ gives a linear relationship between u_1 and elements of ε (in situations where $\partial V / \partial u_1 = 0$ exists).

- Model 3 (Linear in u_1 and d):

The $\langle u_1, u_1 \rangle$ terms are neglected in Eq. (14) and only the linear terms with respect to d in Eq. (22) are included. This model is just the continuum mechanical model that is predominantly used at present in the LDSS modelling context [6].

Even though we do not allow deformations perpendicular to the well, the well material will still be strained because of the way we defined the reference configuration (the well material is, in the reference configuration, deformed by a homogeneous deformation). The strain perpendicular to the well calculated with model 2 has the form

$$\varepsilon_{\perp} = \frac{1}{2} \left(\frac{a^2}{b^2} - 1 \right), \quad (23)$$

where a is the lattice constant of the barrier material and b is the lattice constant of the well material. It has the form

$$\delta = \left(\frac{a}{b} - 1 \right) \quad (24)$$

calculated with model 3. The parameter δ is known as the lattice mismatch. It can be shown that any strain tensor element calculated with model 2 or 3 will be proportional to the strain perpendicular to the well [1], hence, the difference between model 2 and model 3 will always be given by

$$\frac{\varepsilon_{\perp} - \delta}{\delta} = \frac{1}{2} \delta. \quad (25)$$

In order to compare the non-linear model (model 1) with models 2 and 3 we have made a series of calculations. The results of those calculations are given in Tables 1 and 2. The

Table 1
Silicon in Germanium oriented in the [1 1 1] direction

	Model 1	Model 2	Model 3	Error 1–2 (%)	Error 1–3 (%)
$\varepsilon_{ }$	−0.018775	−0.019131	−0.018734	2.0	0.2
$u_{1,x}$	0.05302	0.055494	0.055494	4.7	4.7

The numbers give the strain and internal strain inside the well in the direction of the well (the barrier material is unstrained).

Table 2
Tin in Germanium oriented in the [1 1 1] direction

	Model 1	Model 2	Model 3	Error 1–2 (%)	Error 1–3 (%)
$\varepsilon_{ }$	0.61515	0.060597	0.064747	−1.5	5.3
$u_{1,x}$	−0.20886	−0.19043	−0.19043	−8.8	−8.8

The numbers give the strain and internal strain inside the well.

lattice mismatch δ of the Silicon–Germanium system was 4.2% whereas it was −12.8% for the Tin–Germanium system.

From these results we can draw the following conclusions. First, the error due to the linear approximation of the strain ε is equal to $\delta/2$. Second, the error in the internal strain u_1 due to the linear approximation of u_1 can be higher than the lattice mismatch δ . And third, the error in the strain ε due to the linear approximation of u_1 is not higher than $\delta/2$ at least for the systems under investigation here. There is, however, no reason why this should be the case for an arbitrary material system.

4. Conclusion

In this paper, we have presented a non-linear strain theory for low-dimensional semiconductor heterostructures that is continuous in nature but derived from the atomistic framework and, thus, contains the best of both worlds. Hence, our strain theory includes physically plausible interface boundary conditions. It also explicitly includes the quantity known as internal strain. We have, in addition to this, presented results of strain calculations using the theory developed on two different quantum well systems: Silicon in Germanium and Tin in Germanium. The obtained results have shown that non-linearities can give results that differ from the linear case close to $\delta/2\%$ and that the non-linearities in the internal strain are just as important as the non-linearities in the strain itself.

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