Tutorial 5B
Strain

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**Objective:** Find relaxed positions of atoms

Example: Quantum dot (10M Atoms, 100s CPUs, hours)

Let’s run the input-deck (it will take several minutes)

```bash

cd ~

cd public_examples/NCN_summer_school_2012/Quantum_Dot_Hesam

!ln

Don’t Forget Exclamation Sign!

ln -s /apps/share64/nemo/examples/current/materials/all.mat

submit -v ncn-hub@coates -i ./all.mat -n 8 nemo-r8028 a_QD_10nm_Usman.in
```
Outline

Why do we need relaxed positions?

Strain Examples:
1. Quantum Dot with Open Boundaries
   » Input deck ↔ Flow chart
2. Quantum Dot with all types of boundary conditions
   » How to apply different boundary conditions
3. Quantum well
“Stand up to a Computer”

S. Fergusson, Eng. In Mind’s Eye, MIT Press

Understand how simulation software works
How to obtain the Atoms positions and Strain?

1- Initial Placement of Atoms

2- Minimize Elastic Energy
   Displace atoms

Converged?

No

Yes

3- Calculate Strain

← Here we have final atom positions
Example 1: Quantum Dot with Open Boundary

Input deck ↔ Flow chart
**1st Step:** How to setup initial positions in input-deck?

1. **Initial Placement of Atoms**
   - Minimize Elastic Energy
   - Displace atoms

2. Converged?
   - No
   - Yes

3. **Calculate Strain**

**Structure**
1. Material
2. Domain
3. Geometry

**Solver**
1-a) Materials

- GaAs and InAs
- We can change material properties here
- The regions will be determined in Geometry
Initial positions of Atoms

1-b) Geometry

- dimensions are in nm
- The region numbers are what we specified in material section

Geometry
{
    //--- GaAs Substrate ---\"
    Region
    {
        shape = cuboid
        region_number = 1
        priority = 1
        min = (-0.1,-0.1,-0.1)
        max = (3.5,3.5,3.5)
    }
    //--- InAs Dot ---\"
    Region
    {
        shape = cuboid
        region_number = 2
        priority = 2
        min = (1.13,1.13,1.13)
        max = (2.26,2.26,2.26)
    }
}
1-c) Domain

- **Base material** is very important in Strain simulation.
- It determines the building block of the structure and initial positions of atoms.
- The boundary condition will be applied to these initial positions.

```plaintext
Domain
{
    name = atomic_structure
    type = pseudomorphic
    base_material = substrate
    dimension = (6, 6, 6)
    periodic = (false, false, false)

    crystal_direction1 = (1, 0, 0)
    crystal_direction2 = (0, 1, 0)
    crystal_direction3 = (0, 0, 1)

    space_orientation_dir1 = (1, 0, 0)
    space_orientation_dir2 = (0, 1, 0)
    passivate = false
    origin = (0, 0, 0)
    output = (xyz, coupling)
    regions = (1, 2)
}
```
Base Material:
Initially GaAs and InAs have the same lattice constant

Initial position

GaAs  InAs  GaAs

After strain solver
2nd Step: How to setup Strain solver in input-deck?

1. Initial Placement of Atoms
2. Minimize Elastic Energy
   - Displace atoms
3. Calculate Strain
   - Converged?
      - Yes
      - No

Solver
2) Strain Solver

- **type** determines the solver. For strain solver type should be "KeatingStrain" or "VFFStrain".

- **models** determine the interatomic potential function

Standard Keating: harmonic
Lazarenkova : anharmonic_Areshkin
Modified VFF: cross-stretch, stretch-bend, …
Strain Solver Parameters

**Keating**
Models = harmonic

**Lazarenkova**
Models = anharmonic_Areshkin

Potential $U(r)$

Displacement
Max: 0.2068
Min: 0.0000

Max: 0.2519
Min: 0.0000
3rd Step: Convergence criteria and outputs in input-deck

1- Initial Placement of Atoms

2- Minimize Elastic Energy
   Displace atoms

Converged?

No

Yes

3- Calculate Strain

Solver
Strain Solver Parameters

2) Strain Solver

- **calculate_epsilon**: Enables the strain calculation.
- **absolute_tol** and **relative_tol**: Determine the convergence condition.
- There are different matrix solvers and preconditioners which affect convergence speed.

```plaintext
solver
{
    ...

    // Outputs
    calculate_piezo            = true
    calculate_epsilon          = true
    silo_file                  = Graphic_Output.silo
    xyz_file                   = Text_Output.xyz
    xy_file                    = Text_Output_Strain.xy
    calculate_bond_stats       = Bond_Lengths.bonds

    // Petsc options
    linsolver_max_iters       = 300000
    linear_solver             = bcgs1
    preconditioner            = jacobi
    max_num_iters             = 200000
    absolute_tol              = 1e-8
    relative_tol              = 1e-8
    linsolver_monitor         = true
}
```
Strain Outputs

- Graphic Output (Displacement, Strain)
Exercise: Strain and displacement in Quantum dot

Goal: How to run solver and plot the displacement/strain

Geometry Definition for Strain

2. Quantum Dot with all types of boundary conditions
   » How to apply different boundary conditions
• How to make periodic boundary condition?

```
Domain
{
    name = atomic_structure
    type = pseudomorphic
    base_material = substrate
    dimension = (6,6,6)
    periodic = (true,true,false)  // ---- Periodic in x and y directions
    crystal_direction1 = (1,0,0)
    crystal_direction2 = (0,1,0)
    crystal_direction3 = (0,0,1)
    space_orientation_dir1 = (1, 0, 0)
    space_orientation_dir2 = (0, 1, 0)
    passivate = false
    origin = (0,0,0)
    output = (xyz,coupling)
    regions = (1,2)
}
```
• How to make fixed boundary condition?

Geometry
{
    
    Boundary_region
    {
        shape = cuboid
        region_number = 1
        priority = 1
        min = (-0.1,-0.1,-0.1)
        max = (3.5,3.5,0.1)
    }
}

• All atoms in this volume will be fixed

To fix a boundary

➢ Change in Geometry
Introduce the boundary region

➢ Change in strain solver
Choose the boundary in
fixed_boundary = (1,5,6)
• How to make fixed boundary condition?

```java
solver {
    name = keating
    type = KeatingStrain
    ...
    // Boundary
    fixed_boundary = (1)
}
```

To fix a boundary

- **Change in Geometry**
  Introduce the boundary region

- **Change in strain solver**
  Choose the boundary in fixed_boundary = (1,5,6)
Outputs

- Displacement output
• Example 3: Quantum well
Geometry
{
  //---  GaAs Substrate  ---\\
  Region
  {
    shape = cuboid
    region_number = 1
    priority = 1
    min = (-0.1, -0.1, -0.1) // Units: nm
    max = (4.0, 5.7, 4.0) // Units: nm
  }
  //---  InAs Well  ---\\
  Region
  {
    shape = cuboid
    region_number = 2
    priority = 2
    min = (-0.1, 1.6, -0.1)
    max = (4.0, 3.8, 4.0)
  }
  //---  Left Fixed Boundary  ---\\
  Boundary_region
  {
    shape = cuboid
    region_number = 1
    priority = 1
    min = (0,0,0)
    max = (4.0,0.2,4.0)
  }
}
Outputs

• Displacement

• Strain eyy
Thanks