# Stress State Determination in Nanoelectronic Silicon Devices Coupling COMSOL Multiphysics and a Recursive Dynamical CBED Pattern Simulation

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**Abstract:** Strained technology is being promoted as the best way to extend the performance of semiconductor transistors. An inhomogeneous layer deposited on top of a silicon device can induce a strong modification in the real silicon strain state, and consequently in its electronic performance. Coupling the finite elements analysis done by COMSOL with a recursive CBED and LACBED dynamical simulation, we are able to explain the observed diffraction pattern modification, reconstructing the strain field in the device.

**Keywords:** Strained silicon technology, device, CBED, LACBED, TEM

## 1. Introduction

Strained technology is being promoted as the best way to extend the performance of semiconductor transistors, and the downscaling of the silicon technology continues the shrinking of the device geometry. When the devices are strained by a non uniform stressor source, the usual process device simulators are no more able to describe the strain distribution, and a more accurate description of the resulting strain distribution is required. This is the case of almost all the recent microelectronic devices, where the actual dimensions are reduced down to 45 nm and even below for both memory cell elements and transistor device [1]. To improve their performance, the strained silicon technology is currently used by the electronic industries [2]. The most used stressor sources are either the lateral strain elements (i.e.: SiC or SiGe source and drain contact) or the deposited-on-top stressor layer (i.e.: tensile or compressive nitride layer). An example of stressed device is given in Fig. 1, which shows a sketch of the silicon substrate and the stressor source. The acronym CBED and LACBED refer to two TEM methods of electron diffraction and will explained in the following. The corresponding electronic device is visible in Fig. 2(a) and (b). In this kind of problem, a mere process device simulation is not

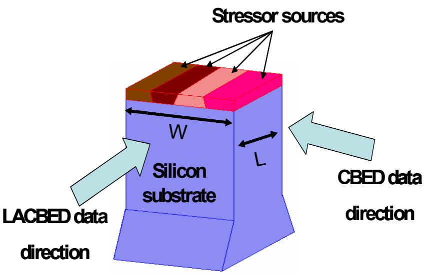

**Fig. 1** A sketch of the analyzed sample, with the stressor sources on top of the silicon substrate

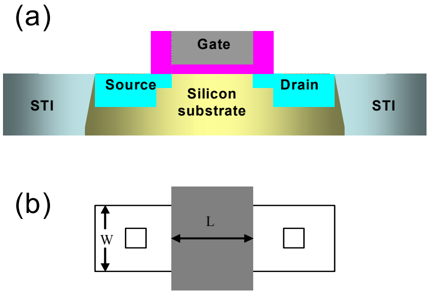

**Fig. 2** A lateral (a) and a top (b) view of the electronic device; the main electronic elements are evidenced, as the geometrical dimensions (width W, length L)

accurate enough to reproduce the strain field, and an experimental method should be employed.

## 2. Experimental problems

It has been recently proved that quantitative strain mapping can be experimental obtained by the Convergent Beam Electron Diffraction (CBED) technique of the Transmission Electron Microscopy (TEM). This technique [3] is based on the analysis of diffraction lines, called HOLZ (High Order Laue Zone), which are very sensitive to the variation in the crystal lattice parameters: a spatial resolution in the nanometre range is feasible, [4], even in the case of highly strained samples [5], like the one presented in Fig. 1. Furthermore, in this case the lines are split in two components, which must be fitted to a computer simulated pattern. To perform the simulations, a model of the induced deformation is needed. We set up a recursive approach, based on the refinement of some parameters involved in the displacement simulation, until the reconstruction of the observed sample is reached.
An experimental view of the stressing layer deposited on top of the substrate is given by Fig. 3: four grain boundary interfaces, generating the displacement field in the underlying silicon, are visible.
In Fig. 4a) is presented an example of experimental pattern, with the corresponding simulation in Fig. 4b).
An additional difficulty is given by the requirement for the TEM/CBED analysis of a thinned sample, that should be transparent to the electron beam. After the thinning, the strain state of the sample can be modified by the elastic relaxation with respect to the original bulk-like case (which is our real interest). Therefore, to reconstruct the real sample configuration before the thinning, we need also additional information from a lateral view, coupled with a recursive simulation of this case. The experimental pattern should be acquired with a bigger field of investigation, while a smaller resolution is allowed.

## 3. Governing Equations

### 3.1 Thin sample strain state

The modeling of the thinned sample starts from the reproduction of the stressor source in the experimental slice.
We modeled the different strain state of the stressor layer onto the silicon substrate using the Structural Mechanics Module. The deformation induced in the silicon substrate by the grain boundaries (shown in Fig. 3) are well described by a lattice mismatch [6]. We reproduced the morphology of the experimental sample observed in the TEM image, then we used a static analysis of a thermal relaxation. We recursively adjusted some selected parameters (thermal expansion coefficients, geometrical parameters) for the various elements involved, in order to reproduce the strain state of the devices. By this way, we obtain the input for the

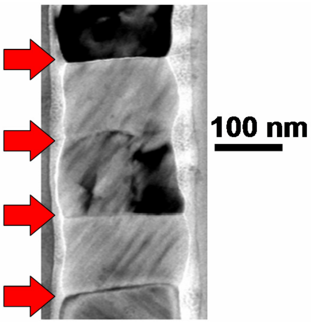

**Fig. 3** A stripe of grain boundary, which are the induced deformation sources. The bamboo-like distribution is clearly visible; four interfaces between adjacent grains are shown by the arrows.

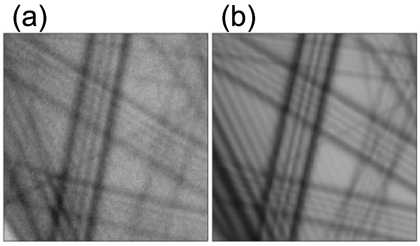

**Fig. 4** a) A detail of an experimental CBED pattern, including split diffraction lines, and b) the corresponding simulation, resulting from the recursive strain field reconstruction.

calculation of the recursive dynamical CBED simulations, in order to reproduce the experimental patterns in the 3D sample.

We started assuming for the stressor source a purely radial shape (and consequently a radial deformation). Then we introduced a more complex ellipsoidal deformation, adjusting the ratio between the semi-axes. The resulting displacement field, obtained by COMSOL, is shown in Fig. 5.

### 3.2 Entire sample strain state reconstruction

After the reproduction of the strain state in the thinned sample, we can initiate the reconstruction of the deformation observed in the thick case. For these case, we should use the experimental information taken from a different view of the sample, acquired with the LACBED (Large Angle CBED) technique [7]. By this method, we can obtain information about the strain state from a larger area with respect to the CBED technique.

Starting from the reconstructed deformation model in the thin sample, we use the experimental data acquired by LACBED in the lateral view to extend the deformation model in the 3D space, again using a recursive method.

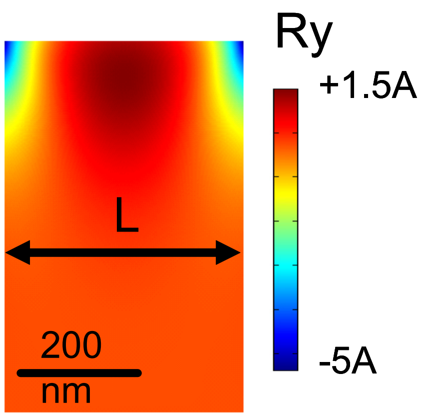

**Fig. 5** Displacement field reconstructed in the thinned sample. The vertical component is shown.

## 4. Theory

The deformation induced into the substrate by the stressor source can be computed by using a pseudo thermal expansion, assuming a lattice mismatch between the grain boundary and the substrate. The induced strain is computed by the following relation:

$$\varepsilon = \alpha \cdot \Delta T$$

where **α** is the thermal expansion coefficient and **ΔT** is the temperature variation. In our case, we use a value of $\mathbf{\Delta T}=1K$, and then we recursively modified the value of the parameter **α**.

The relation between the resulting strain components $\varepsilon_{ij}$ and the displacement is calculated accounting for the large deformation by the Green-Lagrange strain equation:

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial R_i}{\partial x_j} + \frac{\partial R_j}{\partial x_i} + \frac{\partial R_k}{\partial x_i} \cdot \frac{\partial R_k}{\partial x_j}\right) \quad (1)$$

where the $R_i$ represents the displacement components along the $x_i$ directions, and the third term takes into account the non-linearity. After the strain calculation, we compute the stress in the material using the constitutive relation:

$$\boldsymbol{\sigma} = \mathbf{D}\boldsymbol{\varepsilon} \quad (2)$$

where **D** is the 6x6 elasticity matrix and **σ** represents the stress tensor.

## 5. Numerical Model

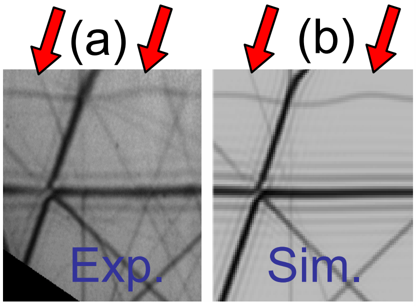

**Fig. 6** a) Experimental, lateral view of the sample. Two bending of the Bragg contour (connected to the deformation induced in the cristallographic plane by the stressor sources) are evidenced by the red arrows. b) Corresponding simulation, obtained by the LACBED simulation after the recursive reconstruction in the thick sample.

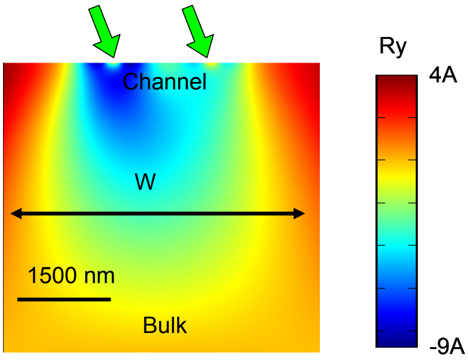

**Fig. 7** The resulting displacement field obtained by the presented method, displayed in the W direction. The green arrows indicate the stressor source on top of the silicon substrate. The current flow occurs on top of the selected region.

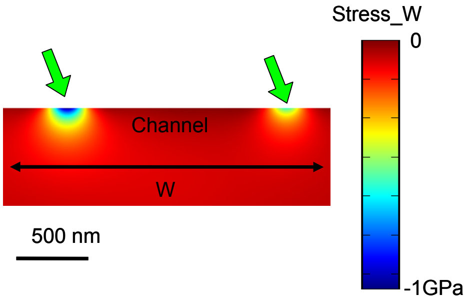

**Fig. 8** The resulting displacement field obtained by the presented method, displayed in the W direction, representing the starting point for the calculation of the mobility variation. The green arrows indicate the stressor source on top of the silicon substrate. A peak of compressive stress up to 1GPa is reached.

The displacement deformation induced into the thin sample are calculated by a 3D geometry, using two different elements: the stressor source and the substrate. The substrate was simulated using the standard silicon properties, with the assumption of the correct anisotropy of the elastic stiffness in the different used directions. The stressor source was modeled with an ellipsoidal shape, inserted on the highest part of the substrate, as presented in the sketch of Fig. 1. Different configurations of the strain source were used, until the observed deformation induced into the substrate are fitted. We analyzed different thinned samples, with thickness in the range between 400 and 500 nm (calculated in the W direction, see Fig. 1). Then we are able to reconstruct the thick sample also in the L direction (Fig. 1).

The bulk-like was simulated with a 3D model, using the same thickness of the thin sample and a L lateral dimension in the micrometer range.

## 6. Results and Discussion

We found that the problem of the strain field generated by a non homogeneous stressor layer in a silicon device can be described by an appropriate series of stressors, with different thermal relaxation parameters.

First, we reconstruct the strained configuration of the thin sample, by using an appropriate recursive simulation code for the HOLZ pattern simulation [8]. The good agreement between the experimental data of Fig. 4 (a) and the corresponding simulation of Fig. 4(b) is evident. The resulting displacement field is given in Fig. 5.

Then, we can reconstruct the complete real sample strain state, using the information of the lateral view to recursively reconstruct the experimental LACBED pattern of the thick sample. The results of the iterative procedure is visible in Fig. 6, which shows the experimental data (Fig. 6a) and the corresponding simulation (Fig. 6b). The resulting displacement field, obtained by the COMSOL simulation, is given in Fig. 7. From these results, the stress configuration close to the interface can be calculated, for both the L and W directions (indicated in the sketch of Fig. 1). By the stress field computation in the region of the channel, the carrier mobility can be evaluated, giving fundamental information about the electronic performance of the devices. [9].

## 8. Conclusions

The various components of the strain field in the active area of a strained silicon device can be obtained, coupling the finite elements analysis by COMSOL with a recursive CBED pattern dynamical simulation. Starting from this stress state results, the carrier mobility variations can be calculated.

## 8. References

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