Materials Science in Semiconductor Processing 87 (2018) 65–68

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

Lattice contraction due to boron doping in silicon

Victor Boureau[a,b], Jean Michel Hartmann[c], Alain Claverie[a,*]

[a] CEMES-CNRS and University of Toulouse, 29 rue Jeanne Marvig, 31055 Toulouse, France
[b] STMicroelectronics, 850 rue Jean Monnet, 38920 Crolles, France
[c] Univ. Grenoble Alpes, CEA, LETI, 38000 Grenoble, France

ABSTRACT

In modern electronic devices, strain is used to increase carrier mobility. It is thus mandatory to know precisely the effect of doping on the lattice parameter of silicon. However, there are many experimental biases which prevent one from measuring this effect with high accuracy. For this reason, we have designed and fabricated a step-like structure consisting of five 50 nm-thick Si layers of increasing substitutional boron concentrations. Then, we have used Dark Field Electron Holography, a Transmission Electron Microscopy based technique, to measure the strain in these pseudomorphic and defect-free layers. Using Finite Element Modelling, we show that the observed out-of-plane strains can be reproduced by assuming that the expansion coefficient of boron is about -6.5×10^{-24} cm^3. This value is slightly larger (in absolute value) than those previously reported. It is otherwise about 20% larger than predicted from the size mismatch between B and Si atoms.

Strain is today an integral feature of modern electronic devices. Indeed, the mechanical deformation of the crystalline lattice modifies the effective mass, the scattering, and consequently the mobility of charge carriers in semiconductors [1]. This principle is being extensively applied to boost the performance of Si and Ge based devices by introducing strain of desired amplitude and direction in the channel region of metal-oxide-semiconductor field-effect transistors [2–4]. There are several different possible technological routes to implement this strain, from the deposition of intrinsically stressed layers such as SiN and TiN to the engineering of sources and drains of different lattice parameters. In the latter case, the short channel region is confined between the two strained pockets and deforms to an equilibrium (strained) configuration which can be predicted using Finite Element Modelling (FEM).

To engineer this strain, source and drain regions can eventually be built of epitaxial alloys such as silicon-carbon (Si_x C_{1-x})[5–8] and silicon-germanium (Si_x Ge_{1-x}) [9–12] of various compositions that have lattice parameters different (smaller and larger, respectively) from those of the Si matrix. The relations between C or Ge concentrations and resulting lattice parameters are well established [13,14]. However, these regions have to be heavily doped. The dopant atoms being of different sizes than the host Si atoms, this substitution will also result in a change of its lattice parameter. Thus, the final characteristics of the channel will also depend on the dopant concentrations in the source and drain regions. The fine tuning of strain in the channel of modern devices thus requires that the impact of doping on the lattice parameter of Si is also precisely established.

Boron being the classical p-type dopant of Si, one might think that the relation between B concentration and lattice parameter is known since decades. Surprisingly, as it will be shown latter in this letter, this is not the case. In general, it is noted that the substitution of silicon by boron atoms results in a contraction of the lattice. In theory, the change of lattice parameter should linearly depend on the boron concentration through β, the expansion coefficient. The simplest approach consists in attributing this change to the difference of atomic radii between the host (Si) and the substitutional impurity atoms (B). This is known as the Vergard's law for solid solutions. For boron in silicon, this leads to an expansion coefficient β of about -5.46×10^{-24} cm^3 (atomic radii from [15]). Actually, a second mechanism may play a role through electronic interactions (deformation potentials) [16], enhancing or reducing the size mismatch effect. A spectacular example of the effect of deformation potentials is that of As, which expands more the Ge lattice than the Si lattice [17].

However, the relation between boron concentration and change of the lattice parameter is often found to be not linear, the contraction appearing proportionally smaller for high boron concentrations. This characteristic evidences the difficulties of running clear cut experiments in that field. Indeed, there are a number of biases which should be avoided to establish an accurate relation between dopant concentration and lattice parameter. Firstly, all impurity atoms should be dopants i.e., they must only sit on substitutional sites and consequently be electrically active. Indeed, inactive boron occupies interstitial sites, alone or in clusters, and tend to strain the Si lattice in the opposite direction i.e., towards a larger lattice parameter. This will mask the contraction effect due to substitutional doping. Secondly, the doped silicon crystal should be defect-free, with no dislocations or Boron Interstitials Clusters

* Corresponding author.
E-mail address: claverie@cemes.fr (A. Claverie).

https://doi.org/10.1016/j.mssp.2018.07.011
Received 6 June 2018; Received in revised form 25 June 2018; Accepted 5 July 2018

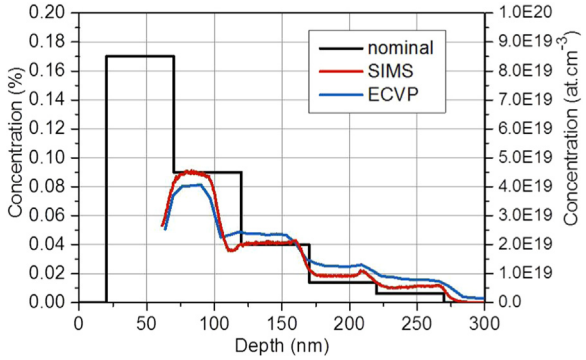

Fig. 1. Boron concentration profiles measured by SIMS and ECVP in the stacked structure plotted together with the nominal concentrations measured by four probes resistivity on full sheet companion samples.

(BICs). Finally, the doped silicon should be homogeneous, as expected for a solid solution. Thus, appropriate samples are hard to fabricate, which probably explains the disagreement between published reports. In this work, we have specially designed and fabricated a sample of high purity and used a combination of experimental techniques to avoid these biases.

A 200 mm Si(100) sample consisting of a stack of five 50 nm-thick doped Si layers of increasing boron concentrations, from 3×10^{18} to 8.5×10^{19} at cm^{-3}, was grown by Reduced Pressure – Chemical Vapor Deposition (RP-CVD) in an AMAT Epi Centura 5200 reactor at 650 °C under conditions favoring the incorporation of boron atoms on substitutional sites during growth (i.e., at 20 Torr with SiH_4, B_2H_6 and high amounts of ultra-pure H_2 as a carrier gas [18]). The doping concentrations were measured by four probes resistivity on companion samples grown as single doped layers under the very same conditions. The stack was finally covered by a 20 nm thick undoped Si layer. The atomic boron concentration depth profile was measured by Secondary Ions Mass Spectroscopy (SIMS) while the carrier concentration depth profile was measured using Electrochemical Capacitance-Voltage Profiling (ECVP) [19]. Fig. 1 shows the results of these measurements.

For the 4 layers up to a concentration of 4.5×10^{19} B cm^{-3}, the SIMS and EVCP profiles are in very good agreement and very close to the nominal concentrations, within $\pm\ 2 \times 10^{18}$ B cm^{-3}. This shows that almost all (if not all) the boron atoms are on substitutional sites in these layers. Close to the surface, both the SIMS and the ECVP techniques show different artifacts which prevent us from absolute comparison. For this layer, we assume that the doping concentration is that obtained from resistivity measurements.

The change in lattice parameter due to doping of the epitaxial layers leads to in-plane stress in the pseudomorphically grown films. In reaction, the films shrink in the perpendicular direction (out-of-plane strain) by an amount that is determined by the local doping concentration and by the elastic constant of Si, through the Poisson's law. In general, these out-of-plane lattice spacing are measured by x-ray diffraction on separate samples. In our work, we have used Dark Field Electron Holography (DFEH) to measure these deformations on the same sample. DFEH is a recently invented Transmission Electron Microscopy (TEM) based interferometry technique able to map strain with a high precision (2.10^{-4} in this work) and nanometer resolution (5 nm in this work) over micrometers wide fields of view [10,20]. In short, two highly coherent electron waves diffracted respectively by a reference (unstrained) zone and the region of interest are forced to interfere in the image plane and form a hologram. The Fourier analysis of these holograms allows one to extract the phase shifts between these waves from which strain along the diffraction direction can be retrieved. By changing the diffraction vector used for imaging, strain can be explored along all directions of the image plane. For details of the technique, the reader is referred to the book chapter by Hÿtch et al. [21].

Fig. 2.a is a map of the in-plane strain observed in our sample. The inset shows the integrated profile of this image along z, the depth into the sample. Neither strain nor defects can be detected in the structure confirming that the layers were pseudomorphically grown on the Si substrate.

Fig. 2.b is a map of the out-of-plane strain. From the substrate, the image tends to get greenish as the layers contain more boron. Again, the inset shows the integrated profile of this image along the z direction. It clearly shows that strain increases from the substrate towards the Si cap layer at the surface.

We now aim at extracting the expansion coefficient from the comparison of FEM simulations with our DFEH measurements. The model first needs to describe our structure as a stack of five pseudomorphic 50 nm-thick layers of different relaxed lattice parameters. These lattice parameters are linearly related to the local concentrations of boron through the relation:

$$\frac{a_{Si:B} - a_{Si}}{a_{Si}} = \beta . N_B,$$

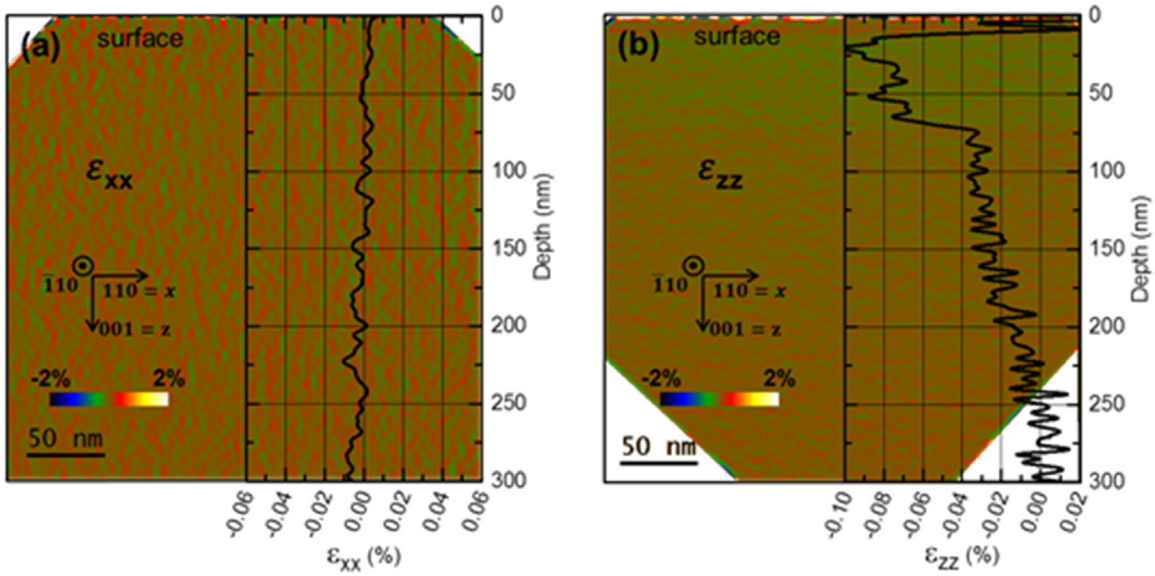

Fig. 2. (a), in-plane (ε_{xx}) and (b), out-of-plane (ε_{zz}) strain maps measured by DFEH. The insets show the integrated strain profiles along the depth of the sample.