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On the use of MEIS cartography for the determination of $Si_{1-x}Ge_x$ thin-film strain

T.S. Avila *, P.F.P. Fichtner, A. Hentz, P.L. Grande

Ion Implantation Laboratory, Institute of Physics, Federal University of Rio Grande do Sul, Av. Bento Gonçalves 9500, CP 15051, CEP 91501-970, Porto Alegre, RS, Brazil

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ABSTRACT

The cartography from MEIS (Medium Energy Ion Scattering) is used to measure lattice deformation of strained $Si_{1-x}Ge_x$/Si heterogeneous epitaxial structures. Higher crystallographic index directions are shown to be specially sensitive to strain leading to a clear quantification of the strain with high sensitivity and accuracy. We provide a simple method to determine the lattice deformation and checked it against full Monte-Carlo simulations. Since MEIS has an excellent depth resolution it can be potentially used to quantify depth-dependent strain in thin-films as well as in nano-structured materials.

1. Introduction

The characterization of the nanoscopic state of strain in crystalline semiconductors is important for distinct applications including, for example, the formation of extended defects [1], the orientation of second phase nano objects [2] or the modification of the valence and conduction band structures and consequently the carrier mobility in semiconducting devices [3,4]. In particular, strained $Si_{1-x}Ge_x$ alloys have been actively investigated during the last years because of their application in high-mobility metal-oxide-semiconductor field-effect transistors [5,6]. The strain appears as a modification in atomic positions. X-ray or electron diffraction have been used to determine changes of the lattice parameter with great precision (better than $\Delta a/a \approx 10^{-3}$) [7,8] and spatial resolution using nano-beam electrons [9]. Micro-Raman and XRD mapping have also been employed to measure lateral strain-field distributions [10]. Quantitative measurements of displacements and strain fields have also been recently demonstrated by scanning Moiré Fringe Imaging in high-resolution scanning transmission electron microscopy [11].

As distinct from diffraction and phase contrast techniques, H and He ion scattering techniques have been extensively employed to determine strain because changes in the channeling or blocking directions [12] can be easily related to lattice deformations [13–16]. Recently medium-energy ion scattering (MEIS) has been successfully used to determine the depth strain profile in thin Si overlayers on SiGe heterostructures [17] and the strain relaxation in GaN/AlN superlattices [18], quantum dots [19], and nanowires [20] among other applications [21–27]. Another powerful ion-beam technique namely High Resolution Rutherford Backscattering Spectrometry (HRRBS) [28], which is comparable to MEIS, has been applied recently to get the strain profile across the HfO_2/Si(001) interface [29]. Most of these methods are based on the determination of the shift in the backscattering yield minima around a given main crystallographic direction using a one-dimensional angular scan. The use of a two-dimensional yield mapping is less frequent but improves the strain measurement [16].

Recently, Jalabert [30] has proposed a new method to evaluate the strain state of a target material called MEIS cartography. In this method the stereographic projection of a single crystal can be measured with a standard MEIS technique for a selected atomic element and depth. Here we demonstrate that this technique can be expanded to characterize strained SiGe heterostructures with high accuracy. In this method, not only the main crystalline directions are analyzed but also the higher index ones. The advantage of this method is its elemental sensitivity with depth resolution and its capability to be used in nano-structured materials. The determination of the strain is based on the position of the many blocking lines contrary to the traditional methods where two directions are used. We also provide a method to determine the lattice deformation fitting the data best and checked it against full Monte-Carlo simulations.

2. Experimental procedure

Metastable $Si_{1-x}Ge_x$ layers with nominal Ge fractions of 20 and 30 at.%, slightly below the critical thickness for pseudomorphic layer growth [31], were grown by molecular beam epitaxy on Si (100) standard wafers [1]. The layers are considered fully strained according to the lattice mismatch predicted by the strain modified Vegard's law [31,32].The thickness of the SiGe layer, stoichiometry and expected out-of-plane strain are depicted in Table 1.

* Corresponding author.
E-mail address: silva.avila@ufrgs.br (T.S. Avila).

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Table 1
Description of samples used in MEIS analysis.

Sample	SiGe thickness	Nominal strain
$Si_{0.7}Ge_{0.3}$	87 nm	2.06%
$Si_{0.8}Ge_{0.2}$	127 nm	1.33%

The MEIS technique is described elsewhere [21,22]. The MEIS measurements were performed using 150 keV He^+ ions provided by a 500 kV electrostatic accelerator from the Ion Implantation Laboratory, Institute of Physics-UFRGS. The samples were mounted in a 3-axis goniometer inside the analysis chamber kept under a pressure of about 10^{-7} mbar. Typical beam current was less than 15 nA. The incidence angle was either 0 and 15° with respect to the surface normal and backscattered He^+ ions emerging from the target were analyzed using a Toroidal Electrostatic Analyzer (TEA) mounted at 120° with respect to the beam direction. At the top end of the TEA a set of two microchannel plates coupled to a position-sensitive detector allows each ion to be energy- and angle-analyzed leading to a two-dimensional (2D MEIS) spectrum, namely a 2D map of ion scattering intensities as function of the backscattering energy and angle. The TEA angular aperture is ~24° and each angle-bin corresponds to 0.08°. The overall energy resolution of the system is ~600 eV. A typical 2D MEIS spectrum obtained for 150 keV He^+ ions impinging on $Si_{0.7}Ge_{0.3}$ sample is shown in Fig. 1. The contributions from He^+ backscattering from Ge and Si are easily distinguished in this figure. Moreover, the reduction of the ion scattering intensity for certain scattering angles (the blocking vertical lines) is also observed. For elements at the surface of the sample (Ge and Si), the signals have different slopes according to the dependence of the kinematic factor on the scattering angle.

In order to measure the stereographic projection of the SiGe samples we followed the procedure described in [30]. In short, a 2D MEIS spectrum is recorded for a series of azimuthal angles (Φ) scanned over typically 60° in steps of 1°. The position of the blocking lines moves as a function of the azimuthal angle. Specifically an energy window is selected, which corresponds to ~1.5 keV wide (about 3 nm at 120°); this signal corresponds to the backscattering yield around a given depth and scattering angle. After integrating the energy bins, a histogram as function of the scattering angle is obtained for each of the scanned azimuth angles. Then a 2D map of ion scattering intensities as a function of the scattering and azimuthal angles can be plotted as shown in Fig. 2. Here the scattering angle (Θ_{sc}) was converted to a polar angle (Ψ) according to $\Psi = \pi - \Theta_{sc} - \Theta_{in}$, where Θ_{in} is the incidence angle with respect to the surface normal direction. Indeed, only part of the stereographic projection can be measured because the angular aperture of TEA is about 24°. However, it can be selected by changing Θ_{in}. Fig. 2a shows the cartography of a standard Si sample using 150 keV He^+ beam close to the Si surface over polar and azimuthal angular ranges of 24 and 60° respectively. The regions with minimal intensities correspond to dark spots and curved-lines and are attributed to the blocking along the principal crystallographic directions and planes respectively. Depending on the direction of incidence and alignment of the sample, channeling effects along the ion beam entrance affect the map and correspond to the black horizontal lines on the map superimposed to the blocking structures. In Fig. 2a the incidence angle is 0° with respect to the normal which leads to a cartography corresponding to the hatched area in the stereographical for Si (see Fig. 2b) taken from Ref. [33].

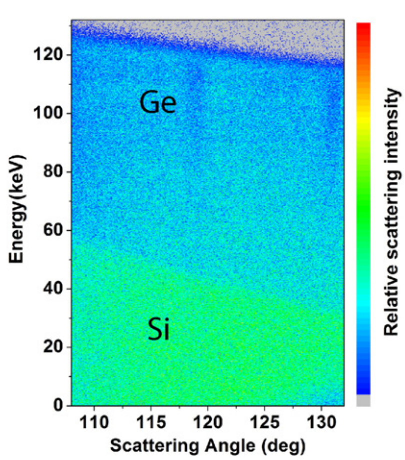

Fig. 1. 2D MEIS spectrum measured with 150 keV He^+ projectiles under normal incidence on the SiGe heterostructure grown over crystal Si. The following signals are observed from top to bottom: Ge and Si from the $Si_{0.7}Ge_{0.3}$, Si from the substrate. Blocking lines in Ge are also visible.

3. Cartography analysis

Position of the blocking spots and lines of a 2D cartographic map, such as the one found in Fig. 2, can be obtained through a simple procedure, based on the definition of a Bravais lattice. Firstly one defines the atomic positions in a conventional cell according to a set of three primitive vectors. Calculations are facilitated if the coordinate system origin is set to the position of an arbitrary atom. By using periodic conditions, a small lattice can be built by creating repetitions of the conventional cell in both positive and negative directions of each primitive vector. The task of finding blocking directions, as a function of polar and azimuth angles, is reduced to looping over all atoms on this reduced Bravais lattice and determining the direction between these atoms and the previously chosen origin. The total number of blocking directions found is related to the number of repetitions applied to the original conventional cell.

The number $N_i(\Psi;\Phi)$ of atoms found along each blocking direction is computed and a corresponding weighting value $w(\Psi;\Phi)$ is calculated:

$$w(\Psi;\Phi) = \sum_{i=1}^{N_i(\Psi;\Phi)} \frac{1}{d_i^2}, \tag{1}$$

where d_i is the distance between the i-th atom in the direction specified by Ψ and Φ and the origin. In general, directions with a large number of atoms present small interatomic distances and consequently a large blocking effect, leading to a relatively large weight w. These are the main crystallographic directions for this particular structure. Fig. 3a shows a crystallographic map for a clean bulk-like terminated Si[100] surface, simulated via the Monte-Carlo MEIS simulation algorithm called VEGAS [35]. Fig. 3b shows the position (open red circles) of blocking directions found superimposed to the simulation just described. The size of each circle is proportional to its weighting value $w(\Psi;\Phi)$, and the matching extends ever to the smaller circles which appear as a red dot.

Fig. 4 shows the cartographic map of a strained-layer $Si_{0.7}Ge_{0.3}$/Si heterogeneous epitaxial structure performed via MEIS with 150 keV He^+ ions and normal incidence; superimposed are the blocking directions found for both relaxed structure (full circles), and for an uniaxial deformation of the unity cell along the sample normal by 2% out-of-plane (open circles). It is interesting to note that both blocking directions seem visually very similar and, indeed, a global shift of 0.48° in the polar angle of the directions of the relaxed structure has the effect of visually reproducing the directions of the 2% strain.

This result creates some ambiguity in the quantification of the strain in a strained-layer, since usually the nominal angles read from the standard MEIS goniometer are known to be not accurate enough. This difficulty can be overcome by either calibrating the polar angles through the use of an unstrained Si reference-sample or by measuring the map over a much wider polar range. Here we used an unstrained Si reference sample in what follows.