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Determination of strain in a buried epitaxial $CoSi_2$ layer in Si(111) by MeV ion scattering and x-ray rocking curve methods

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Abstract : X-ray rocking curve and Rutherford backscattering/channeling techniques have been used to determine the strain in a buried $CoSi_2$ layer of an ion-beam-synthesized epitaxial $Si/CoSi_2/Si(111)$ system. From the x-ray rocking curve, the lattice constant of the buried epitaxial $CoSi_2$ layer has been found to be smaller by 0.78% in the [111] direction compared to the bulk lattice of $CoSi_2$. With ion scattering measurements the tetragonal distortion in the $CoSi_2$ layer was determined to be (1.1±0.2)% and consequently the in-plane strain has been found to be tensile in nature as expected.

Keywords : Epilayer, strain, Rutherford backscattering and channeling, x-ray rocking curve, $CoSi_2$

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1. Introduction

Metallic silicides such as $NiSi_2$ and $CoSi_2$ on silicon substrates are interesting systems both for fundamental research and for applications in microelectronics [1,2]. The low resistivity and higher thermal stability of a $CoSi_2$ layer makes the heteroepitaxial structures of $Si/CoSi_2/Si$ more attractive for their possible applications in high-speed device fabrication [1]. The small lattice mismatch (1.2%) of $CoSi_2$ with substrate Si facilitates the epitaxial growth. Conventionally, molecular beam epitaxy (MBE), solid phase epitaxy (SPE) and reactive deposition epitaxy (RDE) are used to grow epitaxial

silicides. Ion beam synthesis (IBS) is a new method in which a particular type of ions (e.g. Co^+) are implanted into a substrate (e.g. Si) at a high dose. Subsequent annealing of the substrate leads to a reaction between the implanted species and the substrate material resulting in the growth of a buried epitaxial layer of the reacted material (e.g. $CoSi_2$) [3]. The epitaxial silicide layers grow in two possible orientations: type-A, where the silicide layer has the same orientation as the Si substrate, and type-B, where the silicide layer is rotated by 180° about the surface normal of the Si substrate. This orientation of the silicide layer governs the electronic properties of the interfaces (e.g., Schottky barrier height) [4].

For a heteroepitaxial growth, whenever there exists a small lattice mismatch, pseudomorphic growth upto a critical thickness (t_c) is possible as the mismatch can be accommodated by the elastic strain. If the thickness of the epilayer is more than t_c then the strain gets relieved either by introducing misfit dislocations or by shape transition or both [5–7]. Our energy dependent ion channeling measurements showed the existence of misfit dislocations at the bulk $Si/CoSi_2$ interface [8]. The top $Si/CoSi_2$ interface is different as the dechanneling results show the possibility of the presence of stacking faults [9]. The strain in a heteroepitaxial system plays a crucial role. In strained layer superlattice (SLS) structures, one can engineer the band gap by changing the lattice mismatch so as to get the desired physical properties. The strain in epitaxial layers is related to the crystalline quality of the epilayer and the knowledge of strain helps in understanding other physical properties. A complete understanding of the electronic properties is possible only when the detailed structural aspects are known. For our $Si/CoSi_2/Si(111)$ sample, using ion scattering, we determined the thickness, the composition and the crystalline quality of the top Si and the buried $CoSi_2$ layers [10]. Both the interfaces, i.e., the bulk $Si/CoSi_2$ interface and the top $Si/CoSi_2$ interface, have been determined to be of type-A [11]. Also the interfacial atomic structure of the bulk $Si/CoSi_2$ interface was determined with the x-ray standing wave technique [12]. In this paper, we present the detailed study of the strain in the epitaxial $CoSi_2$ layer.

2. Strain in an epilayer

The strain is governed by the lattice mismatch. For a very thin epitaxial layer, the epilayer in-plane lattice constant matches with the substrate in-plane lattice constant when the lattice mismatch between the two materials is reasonably small. Thus for a smaller (larger) lattice constant of the epi-

layer material the layer undergoes a tensile (compressive) in-plane strain and a compressive (tensile) strain in the direction normal to the surface. This mode of growth is called coherent or pseudomorphic growth. The epilayer can grow in the pseudomorphic mode upto the critical thickness t_c. As the layer thickness increases the strain builds up in the layer. For a layer with a thickness larger than t_c, defects – usually misfit dislocations – are generated in the layer in order to relieve the strain.

In Fig. 1, a pseudomorphic and a strain-relieved (via misfit dislocations) epilayer are schematically shown for a system like a $CoSi_2$ layer on a Si(111) substrate. Bulk $CoSi_2$ and Si have CaF_2 and diamond structure respectively. Since the $CoSi_2$ lattice constant is 1.2% smaller compared to Si, in order to achieve the lattice matching with the Si substrate, the $CoSi_2$ layer would have tensile strain within the growth plane ($\epsilon_{\|}$) and compressive strain in the normal direction ($\epsilon_{\perp}$). The strain may be completely relieved for a film thicker than the critical thickness (Fig. 1(b)).

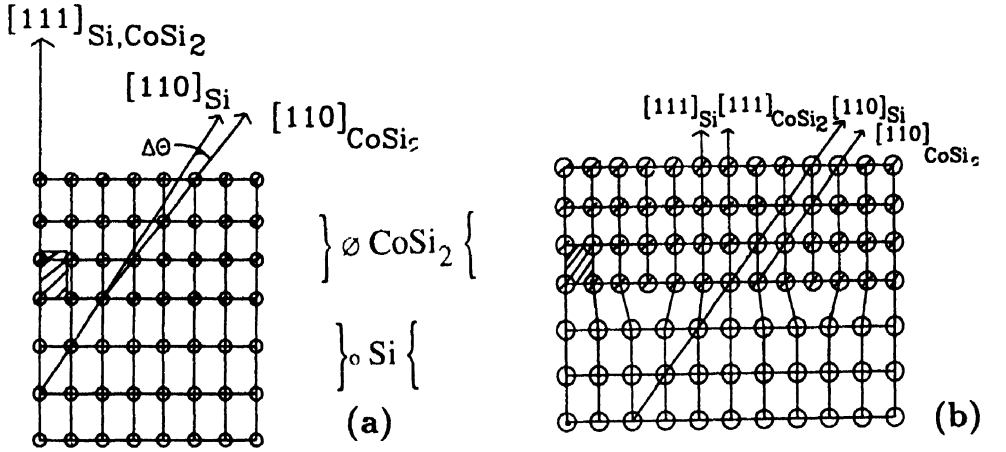

Fig. 1. (a) A pseudomorphic $CoSi_2(111)$ epilayer on a $Si(111)$ substrate; [110] directions are misaligned. (b) A strain relieved $CoSi_2$ epilayer; [110] directions are aligned. The hatched area represents the unit cell of a free $CoSi_2$ lattice.

The two components of the strain are defined as

$$\epsilon_{\perp} = (d_L^{\perp} - d^{\perp})/d^{\perp} \tag{1}$$

and

$$\epsilon_{||} = (d_L^{||} - d^{||})/d^{||} \tag{2}$$

where $d_L^{\perp}$ and $d_L^{||}$ are the interplanar spacing of the strained layer in the direction perpendicular and parallel to the interface respectively. $d^{\perp}$ and $d^{||}$ are the corresponding values for the free lattice of the epilayer material. The tetragonal distortion in the epilayer ϵ_t is related to $\epsilon_{||}$ and $\epsilon_{\perp}$ as follows:

$$\epsilon_t = \epsilon_{||} - \epsilon_{\perp} = \Delta\Theta/(sin\Theta cos\Theta) \tag{3}$$

where Θ is the angle between the [111] and the [110] directions in the substrate (35.26° for Si) and $\Delta\Theta$ is the angular difference between the [110] directions in the substrate and the epilayer [Fig. 1]. Once $\Delta\Theta$ has been determined from the channeling measurement, the value of ϵ_t can be obtained from Eqn. (3). The value of $d_L^{\perp}$ is obtained from the x-ray measurements. With the known value of $d^{\perp}$, $\epsilon_{\perp}$ and $\epsilon_{||}$ can now be determined from Eqn. (1) and Eqn. (3).

3. Experimental

3.1 Sample preparation:

An $Si(111)$ wafer (p-doped) was implanted with 200 keV Co^+ ions to a dose of $2\times10^{17}/cm^2$ while the substrate was kept at 350°C. This was followed by an annealing treatment of one hour at 600°C and 30 minutes at 1000°C to form a 68 nm thick epitaxial $CoSi_2$ layer under an 88 nm of crystalline Si layer [1,10]. Both the epilayers have been found to have the same orientation (type-A) as that of the bulk Si underneath [11].

3.2 X-ray rocking curve measurement:

Recently, an 18 kW rotating anode (Mo) x-ray generator (RIGAKU) has been installed and x-ray rocking curve, x-ray reflectometry and x-ray standing wave facilities have been setup with this x-ray source [12,13]. A highly collimated $MoK_{\alpha 1}$ x-ray beam (λ = 0.709 Å) has been obtained with an asymmetrically cut Si(111) monochromator crystal and used for the rocking curve experiment. The sample is loaded onto the θ-circle of a four-circle diffractometer and the x-ray detector is coupled to the 2θ-circle. The $\theta - 2\theta$ circles are coupled to stepper motors with reduction gears. Fig.2 shows the schematic diagram of the experimental setup. With these stepper motors the minimum angle that can be achieved is 0.001° per step. Initially, θ and

2θ are aligned at zero position and then the detector is moved to twice the Bragg angle ($2\theta_B$) with a wider slit before the detector. Then the angle of incidence θ is varied around the Bragg angle (θ_B) . A part of the data acquisition and control for simple x-ray reflection measurements can be found in Ref. [12]. The complete details about the actual set up will be published elsewhere.

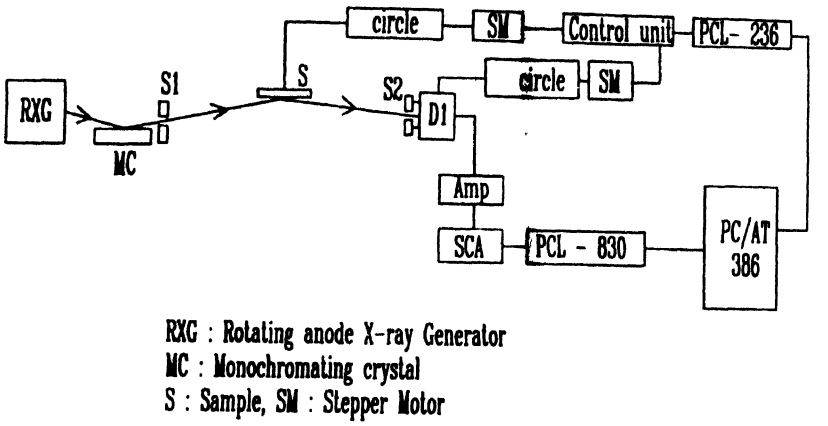

Fig. 2. A schematic diagram of the experimental set-up for x-ray rocking curve experiment.

3.3 Rutherford backscattering and channeling measurement:

He^{++} ions of 3.0 MeV energy were obtained from our 3 MV tandem Pelletron accelerator and used for normal and off-normal axial channeling measurements. The sample was fixed on a goniometer. With the tilt (Θ) and azimuthal (ϕ) angle controls of the goniometer, the [111] crystallographic axis of the sample (along the surface normal) and an off-normal axial direction like [110] were aligned with the incident beam direction. The backscattered ions were detected with a surface barrier detector. The details of this experimental set up are given in references [10] and [14].

4. Results and discussions

The rocking curve from the $Si/CoSi_2/Si(111)$ sample shows bulk $Si(111)$ and $CoSi_2(111)$ diffraction peaks (Fig. 3). The sample is depicted schematically in the inset of Fig. 3. Using the angular difference ($\Delta\theta$) between the diffraction peaks (Fig. 3) and the known (111) planar spacing of bulk Si

(d_{111}^{Si} = 3.135 Å), the (111) planar spacing of the buried $CoSi_2$ layer ($d_L^{\perp}$) can be determined using the relation:

$$\Delta d = -d_{111}^{Si} cot\theta_{111}^{Si}.\Delta\theta \tag{4}$$

where $\Delta d = d_{111}^{Si} - d_L^{\perp}$. Here $\theta_{111}^{Si} = 6.49°$. Eqn. (4) is obtained by differentiating the relation given by Bragg's law: $2dsin\theta = \lambda$. The measured value of $\Delta\theta = 0.132°$ gives $d_L^{\perp} = 3.073 \pm 0.001$ Å. This $d_L^{\perp}$ value is (0.78±0.03)% smaller than the free $CoSi_2$(111) planar spacing($d^{\perp}$). That is $\epsilon_{\perp} = -0.78\%$ (from Eqn. (1)).

The RBS spectra for the random incidence and for an aligned (with [111] axis) incidence are shown in Fig. 4. The backscattering yield is reduced drastically when the incident beam is aligned with an axial direction, because under this condition most of the ions channel into the sample. Fig. 5 depicts the variation of the backscattered He^{++} yield for an incident beam direction around the [110] direction of the bulk silicon. The dips in the angular scan correspond to the [110] crystallographic directions in the bulk Si and the $CoSi_2$ layer. The fact that they do not coincide indicates that the $CoSi_2$ layer is strained. The angular difference between these dips ($\Delta\Theta$) has been found to be $0.3 \pm 0.05°$. From this value the tetragonal distortion (ϵ_t) has been determined to be (1.1 ±0.2)% (from Eqn. (3)). Using the strain in the $CoSi_2$ layer along the surface normal (i.e., $\epsilon_{\perp} = -0.78\%$) and the value of the tetragonal distortion (i.e., ϵ_t= 1.1%), from the Eqn. (3), the lateral strain $\epsilon_{||}$ has been determined to be $(0.3 \pm 0.2)\%$. A pseudomorphic $CoSi_2$ layer should have a value of $\epsilon_{||} = 1.2\%$ and $\epsilon_{\perp}$, according to various estimates, would lie between −0.96% and −2.3% [15]. On the other hand, a fully relaxed $CoSi_2$ layer would have $\epsilon_{||} = \epsilon_{\perp} = 0$. Therefore, the $CoSi_2$ layer in the present study is only partially relaxed. The partial strain relief also indicates the presence of defects at the interface which have been observed for our sample [8]. Our results are in agreement with the earlier works done on similar systems [15-17]. With the assumption that the volume of the strained layer is conserved, a value of $\epsilon_{\perp} = -0.78\%$ would correspond to $\epsilon_{||} = 0.39$, which is within the error bar of our observed value.

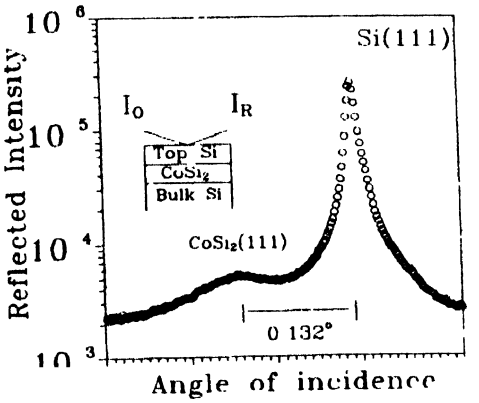

Fig. 3. X-ray rocking curve showing (111) diffraction peaks from a $Si/CoSi_2/Si(111)$ sample. '$Si(111)$' and '$CoSi_2$' represent diffraction from the bulk Si and the $CoSi_2$ layer, respectively.

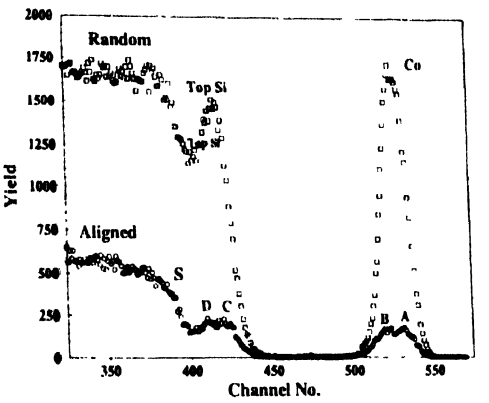

Fig. 4. RBS spectra for random (□) and aligned (○) incidences of a He^{++} beam.

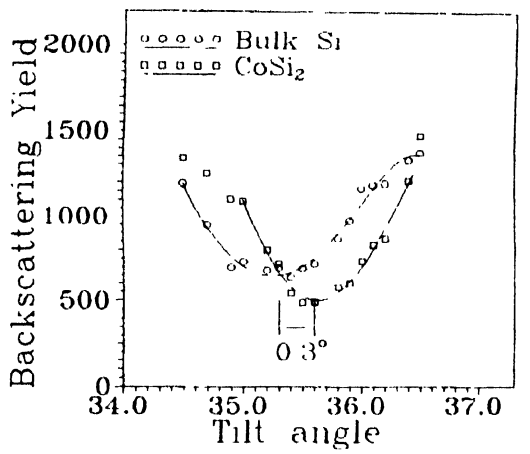

Fig. 5. Variation of backscattering yield of Si in bulk Si and of Co in the $CoSi_2$ layer as a function of tilt angle (Θ) measured from the [111] direction. The minima correspond to the beam alignment with the [110] directions in the bulk Si and in the $CoSi_2$ layer. The misalignment between the [110] directions, $\Delta\Theta$ is 0.3°.

5. Conclusions

We have presented independent determination of both the parallel and the perpendicular components of the strain (i.e., $\epsilon_{\parallel}$ and $\epsilon_{\perp}$) in a buried epitaxial $CoSi_2$ layer by using the RBS/channeling and the x-ray rocking curve techniques. The strain in the buried 68 nm $CoSi_2$ epilayer has been found to be partially relieved compared to a pseudomorphic layer. The measured strain components are in agreement with the idea of volume conservation.

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