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Raman microprobe determination of local crystal orientation in laser annealed silicon

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In this letter we discuss the application of polarization selective Raman microprobe spectroscopy to the detailed, nondestructive analysis of the local crystal orientation of a polycrystalline silicon sample grown over SiO₂ pads and laser annealed. Intensity measurements taken as a function of input polarization angle are fit to an expression derived from the Raman scattering selection rules to calculate the angles by which the crystal structure is twisted within the original substrate plane, as well as the degree of tipping of the crystal plane away from the plane of the Si substrate.

PACS numbers: 61.50.Jr, 78.30.Gt, 81.10.Bk, 63.20. — e

The potential of silicon-on-insulator devices in very large scale integrated (VLSI) architecture¹ has stimulated investigation of methods of growing good quality single crystal silicon on SiO₂ substrates. If the crystal quality is compromised during the growth process by the presence of grain boundaries and similar defects, the electrical properties of the devices being fabricated may be adversely affected.² Hence a rapid nondestructive determination of the local crystal orientation in the material after processing would be of considerable value in the development of silicon-on-insulator devices.

In this letter we discuss the application of polarization selective Raman microprobe spectroscopy to the detailed, nondestructive analysis of local crystal orientation with 1- μ m spatial resolution. This determination depends upon the selection rules³ governing the expected intensity of Raman scattering from Si (cubic O_h crystal point group) as a function of the polarization of the initial light beam relative to the crystal axes. To this end, the Instruments S/A, Inc. microprobe apparatus was modified as in Fig. 1. Samples were obtained by laser annealing of polycrystalline silicon over oxide pads⁴ as briefly described below.

Sample preparation began by depositing a 2- μ m layer of SiO₂ onto a single crystal {100} Si wafer by means of low pressure chemical vapor deposition (LPCVD). The SiO₂ was then patterned into rectangular pads⁴ ranging up to 1 mm in size. A "selective epi" process⁵ was then used to deposit 2 μ m of epitaxial Si in the channels between the pads, so that the planarity of the surface was restored. This was followed by an additional 2 μ m epitaxial growth over the Si regions only, while simultaneously growing 2 μ m of polycrystalline silicon over the SiO₂ pads [see Fig. 2(a)]. The patterned sample was then annealed at a scan rate of 3 cm/s using a 17-W Ar⁺ shaped laser beam with an oval cross section having axes of 80 and 30 μ m. The substrate temperature was kept at 450 °C. A grid array of etch pits was then applied to the surface (see Fig. 1) using a crystal selective chemical etch.⁶ Each pit is about 10 μ m on a side, with diagonals parallel to the <100> directions (see inset Fig. 1). The presence of numerous grain boundaries is apparent.

Figure 2(b) shows the peak intensity of the Si phonon line at 520 cm⁻¹ at two input polarizations of 0° and 90° with respect to the fixed analyzer direction as the sample was stepped at 3- μ m intervals parallel to the etch pit array. The

scattering intensity at each point for 5145 Å excitation as shown in Fig. 2 was measured for values of the input polarization varying at 15° intervals from -75° to 165°. These data were corrected for the polarization dependent response of the beamsplitter which was determined by directly measuring the power on the stage as a function of the input polarization angle. Such corrections involve both an intensity variation and an angle dependent effective rotation of the input electric vector at the sample. By using a single fixed scattering direction, the need for corrections to the scattered transmission is avoided. A detailed exposition of the method of correction will be published elsewhere.⁷ The uncertainty in measured intensity is less than the size of the symbols. Reproducibility is indicated by the repeated measurement at

FIG. 1. Experimental setup. The Ar⁺ laser is tuned to the 5145-Å line; the beam is focused with a $\times 80$ objective to form a spot with diameter on the order of 1 μ m on the sample. The direction of the electric vector of the incident laser beam in the plane of the microscope stage is controlled by the polarization rotator. The sample can be translated using a computer controlled Klinger stage (model UT10025) with a reproducible positioning resolution of 0.1 μ m. The Raman scattered light is collected by the objective and is directed through a fixed polarization analyzer and subsequently into a double monochromator whose output is detected by a photomultiplier. Not shown is a (Coherent model 307 A) noise reduction system placed between the laser and the polarization rotator which is used to keep the input power on the stage constant to within 0.01% over the duration of the experiment. The inset shows the etch pit pattern of the sample; the arrow shows the position and direction of scanning, which is parallel to the direction of laser annealing. This direction is also parallel to the axis of the analyzer. Each pit is 10 μ m on a side.

FIG. 2. (a) Cross section of laser annealed sample. (b) Raman intensity at 3- μm intervals for two different input polarizations separated by 90°. Data have been corrected for the variation of the laser intensity on the microscope stage as a function of polarization angle. (c) Euler angles, calculated from the polarization data at each point, describing the orientation of the local crystal axis system defined by the $\langle 001 \rangle$ directions relative to the laboratory frame defined by the incident laser direction and the fixed analyzer polarization direction.

60 μm . The beam was refocused at each point to avoid spurious intensity variations caused by surface roughness.

Using the Raman selection rules,³ the expression for the scattering intensity I may be found as a function of the input polarization vector angle θ_i and the three Euler angles⁸ α , β , and γ relating the laboratory axis system to the local crystal axis system defined by the $\langle 100 \rangle$ axes. It is given by

$$I \propto [(\mathbf{R}(\alpha, \beta, \gamma) \mathbf{e}_i(\theta_i))^T \chi(\mathbf{R}(\alpha, \beta, \gamma) \mathbf{e}_s(\theta_s))]^2,$$

where $\mathbf{R}(\alpha, \beta, \gamma)$ is a standard rotation matrix⁷ relating the laboratory and crystal axis coordinate systems, $\mathbf{e}_i(\theta_i)$ and $\mathbf{e}_s(\theta_s)$ are the unit vectors in the incident and scattering directions respectively, and χ is the polarizability tensor for the particular phonon symmetry. When the $\{001\}$ plane coincides with the substrate plane, the full expression⁷ reduces to the function⁹ $N \cos^2[2\delta + \theta_i]$, where $\delta = \alpha + \gamma$. Normalization is with respect to the absolute scattering cross section, apparatus collection efficiency, and laser intensity. This simple expression is in excellent agreement with the data at the first spatial point, which is well within a region where $\{100\}$ silicon was epitaxially grown.⁵ After subtraction of the polarization dependent background, the data at all points have been normalized to the value of N at this first point found from fitting to the simplified expression given above. The normalized data at each point were then fit to the general expression, and the angles are presented in Fig. 2(c). Again the reproducibility can be noted by the dual values calculated and plotted for each angle at 60 μm . Uncertainty

in the fits is generally of the order of $\pm 3^\circ$.

The angle β measures the tipping of the $\{001\}$ plane away from the substrate plane. For positions up to 33 μm , $\beta = 0$, indicating no tipping. In this case, δ gives the angle the $\langle 100 \rangle$ crystal axes make with the axis of the analyzer; this sum (modulo 180°) was found to be $(46 \pm 2)^\circ$. This is in agreement with the fact that the projected analyzer axis lies nearly parallel to one side of the etch pits ($\langle 110 \rangle$ direction).

At 36 μm , which is within 2 μm of the edge of the oxide pad, the Raman intensity exhibits a slight rise in both polarizations shown in Fig. 2(b); in Fig. 2(c), β increases slightly to $(8.3 \pm 2.5)^\circ$. At the same time, α and γ both change, but their sum δ remains constant; for small β , the simplified expression still holds approximately. At 45 μm , approximately 10 μm from the pad edge (see inset Fig. 1), the Raman scattering intensities corresponding to the input polarizations shown undergo a strong reversal; this is accompanied by an increase of the tipping angle β to $(38 \pm 2)^\circ$. At 57 μm , β has decreased to a value of about 21° , which is maintained until the intensities of Fig. 2(b) again undergo a reversal. Correspondingly, δ is approximately constant at 6° in this region. If we use the approximation that δ still gives the in-plane rotation angle even for tips of $\beta \approx 20^\circ$, the change in δ corresponds to a rotation of about 45° . This is confirmed by a corresponding rotation of the severely distorted etch pits in this region (see Fig. 1). At the point of the second reversal of intensities (93 μm), β rises to a maximum value of $(45 \pm 2)^\circ$, and for the remainder of the scan always remains above 24° .

The data used here were taken at a fixed wavelength at the peak of the phonon line, with 5.5-cm^{-1} monochromator slit widths. The possibility exists of spurious effects caused by phonon line shifts resulting from strain in the crystal.¹⁰ This was investigated by narrowing the slits and taking a full wavelength scan at 0.1-cm^{-1} intervals over the phonon line at each point shown in Fig. 2. Included in each wavelength scan was a spectral calibration line from an atomic lamp. These data were analyzed by fitting to a Lorentzian convoluted with the slit function of the monochromator to give the width and position of the line with an uncertainty of 0.1 cm^{-1} . A gradual peak shift of $\approx 1\text{ cm}^{-1}$ was observed over the region scanned, small compared with the effective linewidth with the widened slits. The ratio of peak intensities at 0° and 90° was identical in the abbreviated procedure and the full wavelength scans.

The data required for the detailed analysis of the crystal structure presented in Fig. 2 can be obtained rapidly as well as nondestructively. The complete phonon intensity data as a function of input polarization at a single spatial position can be acquired in about 30 s. No sample preparation is required, and all measurements are made at ambient pressure and temperature. In this work, the material is sampled to a depth of about 1 μm , which is the absorption depth of Si at 5145 Å.¹¹ Since the absorption depth is a function of wavelength,¹¹ it can be changed by tuning the Ar^+ laser to other frequencies. The Raman technique can be used with optically thin overlayers, and thus can be applied to encapsulated samples without stripping. In contrast, electron channeling,¹² which can determine angular distortions quickly and to an accuracy of less than a degree, is more of a surface

probe, since it samples only to a depth of $0.05\ \mu\text{m}$. The surface must be cleaned preparatory to placing in a vacuum chamber. A recent report¹³ of a microprobe x-ray diffractometer apparatus apparently obviates the need for a vacuum chamber, but the focused beam size is $30\ \mu\text{m}$, an order of magnitude greater than the focused laser beam used here. The Raman microprobe analysis of crystal structure may therefore have application as a fast test procedure in manufacturing processes since no special handling is needed, while the spatial resolution is of micron dimensions.

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Determination of carrier collection length and prediction of fill factor in amorphous silicon solar cells

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Using a carrier collection length l_c , defined for penetrating light, a convenient technique for measuring l_c in *pin* cells is demonstrated. We show experimentally that l_c predicts the fill factor measured with white light under AM1 conditions for a wide variety of *pin* cells. A simple model is presented which fits the experimental results. The implications of these results on the carrier collection loss for strongly absorbed light are discussed.

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Attempts to increase the efficiency of amorphous silicon *pin* solar cells generally fall into the independent categories of increasing open-circuit voltage V_{oc} , short-circuit current J_{sc} , and fill factor FF. The fill factor is most sensitive to the quality of the *i* layer. In *a*-Si, where the diffusion length is short, the electric field in the *i* layer is primarily responsible for the collection of carriers. As the solar cell is forward biased, the internal field decreases, thereby reducing the carrier collection. It is this effect which limits the fill factor in *a*-Si solar cells, rather than the dark current as in single crystal silicon solar cells. Detailed computer simulations of transport in *a*-Si exist,^{1–3} but there is a need for simplified analytical expressions which can be easily related to experimental measurements. In some models,^{4–8} the electric field does not extend across the *i* layer and carrier collection occurs mainly in the depletion region, although some carriers may diffuse to the high field region. In other models⁹ the electric field is assumed to extend through the *i* layer so that diffusion is not important.¹⁰

In this letter we assume that the electric field is nearly uniform throughout the *i* layer so that a fundamental param-

eter, the collection length l_c , can be defined from a solution of the transport equations. We show how l_c can be easily determined from a single measurement on a completed cell and then used to accurately predict the measured fill factors for a wide class of *pin* solar cells.

The assumption of a substantially uniform electric field across the *i* layers limits the amount of space charge which may be present to approximately less than $2 \times 10^{15}/\text{cm}^3$ for a $0.5\text{-}\mu\text{m}$ -thick *i* layer. In addition, we assume a single set of recombination centers situated near midgap and apply the regional approximation to the recombination rate⁹ to derive a simple expression for the carrier collection ratio η . η is defined as the fraction of the electron-hole pairs collected in the external circuit, divided by the number of photo-generated electron-hole pairs in the *i* layer. η is a function of the wavelength of the light, and the voltage externally applied to the *i* layer. Under these conditions and for penetrating (long wavelength) light, we can write⁹

$$\eta = l_c/L [1 - \exp(-L/l_c)], \quad (1)$$

where l_c is the collection length and L is the *i* layer thickness.