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Evidence from ion channeling images for the elastic relaxation of a $\text{Si}_{0.85}\text{Ge}_{0.15}$ layer grown on a patterned Si substrate

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We demonstrate the ability of ion channeling analysis using a scanned, focused, 2 MeV proton beam from a nuclear microprobe to detect and quantify elastic relaxation in a $\text{Si}_{1-x}\text{Ge}_x$ layer grown on a Si substrate. Channeling images of a sample consisting of a $\text{Si}_{0.85}\text{Ge}_{0.15}$ layer grown on a substrate patterned to produce 10 μm wide raised mesas were produced which revealed lattice plane bending of up to 0.25° , consistent with elastic relaxation of the epilayer. The channeling results are compared with those produced from electron backscattering diffraction. © 1995 American Institute of Physics.

Silicon–germanium alloys grown on silicon substrates offer the potential for the production of fast transistors and novel electronic devices that cannot be produced in unalloyed silicon.¹ The $\text{Si}_{1-x}\text{Ge}_x$ layer has a larger bulk lattice parameter than that of the Si substrate on which it is grown. If the layer is grown below a certain critical thickness, it adopts the substrate lattice parameter in the plane of the interface, resulting in compressive strain along directions in this plane. However, if the layer is grown beyond a critical thickness, it is energetically favorable for some of the strain to be relaxed by the production of misfit dislocations^{2,3} at the layer–substrate interface.

It has been suggested^{4,5} that relaxation of the strained layer through the production of dislocations may be avoided if the layer is grown on to a substrate with a restricted lateral area. Restricted area growth can enable the layer to relax elastically along directions in the interface plane, reducing the strain to below that at which dislocations are produced. It was calculated that for a $\text{Si}_{0.85}\text{Ge}_{0.15}$ layer, restricting the growth area to less than $5\ \mu\text{m} \times 5\ \mu\text{m}$ would enable sufficient elastic relaxation to occur to prevent dislocation production regardless of the layer thickness.⁴ Experimental investigation of $\text{Si}_{1-x}\text{Ge}_x$ growth on isolated substrate mesas has been made using chemical etching and Nomarski optical microscopy⁶ and electron channeling contrast imaging⁷ for samples very similar to that studied in this letter. An absence of misfit dislocations in mesas with widths less than 10 μm was found, and this was attributed to elastic relaxation of the layer on the mesa surface.

In this letter we present direct evidence produced using ion channeling analysis for the elastic relaxation of a $\text{Si}_{0.85}\text{Ge}_{0.15}$ layer grown on to a silicon substrate patterned to produce mesas. Recently, it has been demonstrated^{8,9} that use of a scanned, focused MeV proton beam enables channeling images to be produced of single crystal defects, such as dislocations and stacking faults, using a technique called channeling scanning transmission ion microscopy (CSTIM). This present study demonstrates the ability of ion channeling to characterize the phenomenon of elastic relaxation in micron-size areas.

The samples investigated consisted of an (001) silicon wafer on which square and rectangular mesas were fabricated. A nominally 0.75 μm thick layer of $\text{Si}_{0.85}\text{Ge}_{0.15}$ was then deposited by molecular beam epitaxy so as to cover the mesa and nonmesa areas. Previous studies^{8,10} revealed a dislocation network at the layer–substrate interface both away from the mesas and in the larger mesas. Bunches of these 60° misfit dislocations were imaged by the CSTIM technique, and contrast changes exhibited by the bunches on tilting the crystal so that the incident beam went through the channeling direction were explained using a low-angle grain boundary model.

For this study the sample was mechanically thinned and polished from the back surface to a thickness of about 20 μm and mounted on a goniometer in the Oxford nuclear microprobe.¹¹ The thinning process was not considered to effect the relaxation within the $\text{Si}_{0.85}\text{Ge}_{0.15}$ layer since the substrate thickness is still much greater than the mesa heights on this sample. The 2 MeV proton beam was focused to a spot size of about 300 nm on the sample surface with a

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convergence angle of 0.02° . This was small compared to the measured half-width-at-half-maximum, $\psi_{1/2}=0.2^\circ$, of the channeling critical angle for tilting the sample about the $[001]$ axis in the $(\bar{1}10)$ planes.⁸

The energy loss rate of channeled ions is lowered by a factor of about 2 compared with that of nonchanneled ions. The channeling process is affected in regions of a crystal where the lattice is disrupted by defects or strain so that the ion energy loss rate is locally changed from that produced by perfect crystal. Ion channeling images were produced by measuring the energy loss of protons transmitted through the crystal with the incident beam aligned with, or close to, a channeling direction. Images consisting of 256×256 pixels and showing the mean transmitted proton energy loss were produced by raster scanning the beam over the sample.^{8,10}

Shown in Fig. 1(a) is a secondary electron image of a single $10 \mu\text{m}$ wide mesa. The mesas were $3 \mu\text{m}$ high. Figure 1(b) shows a CSTIM mean energy loss image of a similar mesa. The CSTIM gray-scale images presented here are printed with darker greys representing higher energy loss. This image was taken with the sample tilted so that the beam was 1.0° about each of the two goniometer axes from the $[001]$ axis. This is therefore a nonchanneled image of the mesa, which is showing almost uniform contrast.

The images shown in Figs. 1(c)–1(f) are of the same mesa with the beam at, or close to, the $[001]$ axis. In each of the images, the mesa is showing nonuniform contrast. In particular, one portion of the mesa (arrowed in each image) is lighter than the rest, meaning that the protons were transmitted through this region with a lower mean energy loss. The effect is due to channeling, as it is not revealed in the nonchanneled mesa image of Fig. 1(b). Different regions of the mesa produced a local increase in channeling depending on the angle of the incident beam. It is considered that this effect was caused by the (110) and $(\bar{1}10)$ lattice planes in the alloy layer on the mesa being bent with respect to the corresponding planes in the substrate. It is known from CSTIM studies of misfit dislocations in $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ crystals^{8,10} and Monte Carlo channeling computer simulations¹² that local lattice plane rotation in the top layer of a crystal can shift the angle at which channeling occurs away from the substrate channeling direction.

From Fig. 1, it can be seen that the lattice plane bend angle of the $\text{Si}_{0.85}\text{Ge}_{0.15}$ layer was a function of lateral position on the mesa. From the way that the sample was tilted to produce the images, it can be determined that the (110) and $(\bar{1}10)$ lattice planes in the top layer of the mesa were bent outward from the mesa center. This is the correct sense for the lattice plane bending if the alloy layer on the top of the mesa had relaxed elastically in order to accommodate the misfit strain, as shown below in the insert in Fig. 2(b). An image (not shown) of several small mesas, varying in size from $2.5 \mu\text{m}$ wide to $10 \mu\text{m}$ wide, showed that corresponding positions in each of the mesas permitted the best channeling, suggesting that the lattice planes were bent in the same sense in the layer on each of the mesas.¹³ It is therefore considered that the lattice plane bending revealed in Fig. 1 is a general characteristic of the way that the alloy layer was

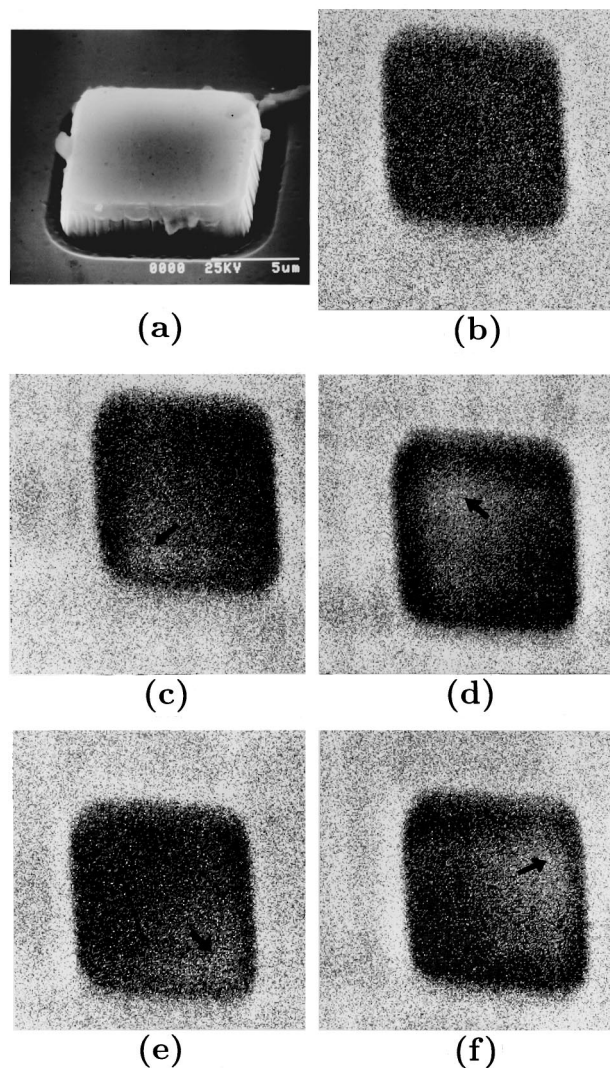


FIG. 1. (a) Secondary electron image of a $10 \mu\text{m}$ wide mesa. Horizontal image width is $16 \mu\text{m}$. (b)–(f) CSTIM mean energy loss images of a $10 \mu\text{m}$ wide mesa with the beam incident at different angles to the (110) and $(\bar{1}10)$ lattice planes. The tilt angles from the $[001]$ axis about the horizontal and vertical directions (θ_x, θ_y) are (b) $(-1.0^\circ, -1.0^\circ)$, (c) $(-0.3^\circ, 0.0^\circ)$, (d) $(0.0^\circ, 0.0^\circ)$, (e) $(-0.3^\circ, -0.3^\circ)$, (f) $(0.0^\circ, -0.3^\circ)$. The sample $[110]$ and $[\bar{1}10]$ directions, respectively, run from left to right and from bottom to top of the images. The arrow in (c)–(f) points to the region of the mesa producing the best channeling.

able to relax for small area growth, consistent with elastic relaxation.

Shown in Fig. 2(a) is a set of horizontal linescans across the center of a single $10 \mu\text{m}$ wide mesa extracted from CSTIM mean energy loss images as a function of sample tilt angle from the $[001]$ axis. The region producing the lowest mean transmitted energy loss, which would correspond to a bright region in a CSTIM image, moved from right to left across the mesa as the beam went from a positive to a negative tilt angle.

From these linescans the amount of bending of the (110) planes on the top of the mesa as a function of position from the mesa center can be determined in conjunction with previous Monte Carlo computer simulations¹² made using the computer code FLUX3.¹⁴ These simulations assumed a $20 \mu\text{m}$

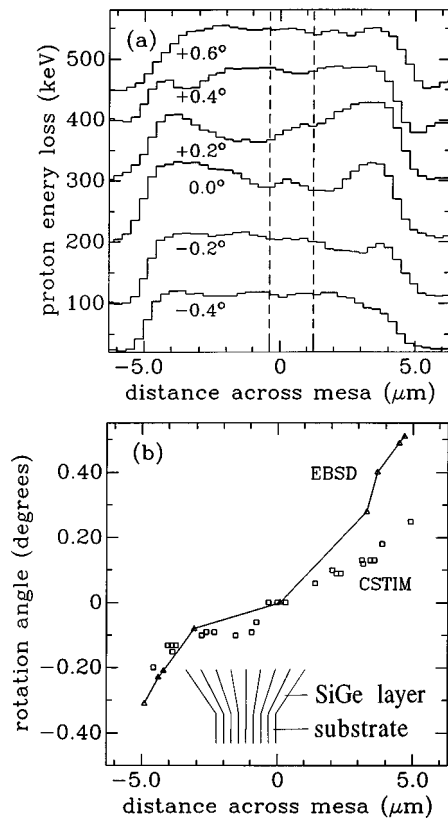


FIG. 2. (a) CSTIM mean energy loss linescans extracted from a single $10\ \mu\text{m}$ wide mesa as a function of beam angle to the (110) channeling planes, whilst still channeled in the (1 $\bar{1}$ 0) planes. Each curve is plotted with the background energy loss subtracted so that the value away from the mesa is set to 0 keV. The curves have been offset vertically by an additional 100 keV from each other and the beam angle to (110) is given. The region between the two vertical dashed lines marks the location of one or more dislocations and is not used to calculate lattice bending angles. This region is probably responsible for the measured asymmetry in the bend angle across the mesa shown in (b). (b) Plot of the lattice bending angle vs distance from the mesa centered deduced from CSTIM linescans extracted from four similar $20\ \mu\text{m}$ wide mesas (square data points). Also plotted are the bend angle values found from a similar mesa by the EBSD technique (triangular data points). The error on the CSTIM and EBSD points is 0.03° . The insert shows the sense in which the lattice planes are bent.

thick crystal which had the lattice planes in the top $1\ \mu\text{m}$ bent by an amount δ with respect to the substrate planes. The transmitted proton energy was found as a function of sample tilt angle θ about the (110) planes for various values of δ .¹² The lateral positions on the mesa where the proton energy loss is locally lowered in the linescans of Fig. 2(a) enable values to be deduced for the lattice plane bending angle across the mesa using the simulated curves. It is recognized that this analysis does not take into account the dependence of the $\text{Si}_{0.85}\text{Ge}_{0.15}$ layer bend angle with height above the layer interface, and it assumes that the resultant dechanneling behavior can be adequately characterized by an abrupt, rotated layer interface.

Figure 2(b) shows the lattice plane bending angle versus lateral distance from the center of four similar $10\ \mu\text{m}$ wide mesas, using this method of analysis. The data points from all four mesas lie well on a single curve, showing that the lattice plane bending behaved in a similar manner in each. The bending is close to zero near the mesa center and in-

creases at a rate of approximately 0.05° per micron to a value of 0.2° at $4\ \mu\text{m}$ from the mesa center. Also shown in Fig. 2(b) are values measured from EBSD patterns⁷ for a $10\ \mu\text{m}$ wide mesa taken from the same wafer used to produce the ion channeling results. The EBSD angles are for the bending of the (102) zone axis across the mesa. In order to compare the EBSD results with the CSTIM (110) plane bending angles, it is necessary to assume that the strain relaxation is uniform across the mesa width; however, the slight asymmetry in the EBSD curve suggests that some strain variation is present. The EBSD results show a similar rise in lattice plane bending with distance from the mesa center, but give a higher value than CSTIM for the bending angle near the mesa edge. This is most likely to be due to the different analytical depths of the two techniques. The EBSD technique samples the lattice plane bending in the top 20 nm or so of the sample, whereas CSTIM is sensitive to the lattice plane bending throughout the whole depth of the epilayer. Since the lattice plane bending would be expected to be greatest near the sample surface, the EBSD technique would be expected to produce a greater value for the bending angle than CSTIM. It is also possible that the assumption in the channeling simulation model of an abrupt bending of the lattice planes in the layer will lead to an underestimate of the plane bending angle in the layer on the mesa using the CSTIM technique.

In conclusion, elastic relaxation of strained layers grown on to restricted area substrates has, for the first time, been demonstrated using transmission ion channeling images. Direct observation of the effect has allowed values for the lattice plane bending in the epilayer to be deduced which are in reasonable agreement with EBSD results. This work thus significantly advances the capabilities of ion channeling analysis since it shows that direct measurement of the elastic strain across micron-size areas can be made.

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