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To cite this version:
M. Wilson, P. Ashburn, B. Soerwirdjo, G. Booker, P. Ward. TEM AND RBS STUDIES OF THE REGROWTH OF ARSENIC IMPLANTED POLYSILICON DUE TO AN OXIDATION DRIVE-IN. Journal de Physique Colloques, 1982, 43 (C1), pp.C1-253-C1-258. <10.1051/jphyscol:1982135>. <jpa-00221792>

HAL Id: jpa-00221792
https://hal.archives-ouvertes.fr/jpa-00221792
Submitted on 1 Jan 1982

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TEM AND RBS STUDIES OF THE REGROWTH OF ARSENIC IMPLANTED POLYSILICON DUE TO AN OXIDATION DRIVE-IN


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Résumé Des couches de silicium polycristallin de 140nm d'épaisseur ont été déposées sur des lames de silicium d'orientation (100), implantées avec des ions arsenic (40keV, 5 x 10^{15} cm^{-2}) et recuites sous atmosphère sèche d'oxygène à 1000°C. Des études par microscope electronique en transmission et par rétrodiffusion de particles a ont montré qu'initiallement les grains croissent, puis qu'ensuite ils recrystallisent en donnant un matériau monocrystallin. Le temps pendant lequel la recrystallisation s'effectue dépend du traitement appliqué à la lame de silicium immédiatement avant la déposition du silicium polycristallin. Les structures obtenues et les distributions en arsenic sont décrites et discutées.

Abstract Polysilicon layers 140nm thick were deposited onto (100) silicon slices, implanted with 5 x 10^{15} cm^{-2}, 40keV arsenic ions, and given a dry oxygen drive-in at 1000°C. TEM and RBS studies showed that the polycrystalline grains initially coarsened and subsequently regrew to give single-crystal material. The time taken for the regrowth to occur depended on the treatment given to the silicon slice immediately prior to the polysilicon deposition. The resulting structures and arsenic distributions are described and discussed.

1. General The deposition of a polysilicon layer onto a single-crystal silicon slice, followed by ion implantation of a dopant and an oxidation drive-in, is of interest with regard to both MOS and bipolar integrated circuit fabrication. In the present work, n-type (100) silicon slices were given a blanket boron deposition treatment similar to that used in the fabrication of standard bipolar transistors. The resulting slices were subjected to either a 10s etch in a CF_{4} plasma or a 10s, dip-etch in buffered HF, and this was immediately followed by the deposition at 620°C of an undoped polysilicon layer \( \approx 0.14\mu m \) thick using a low-pressure chemical vapour deposition method. The aim of these etching treatments was to remove any thin surface oxide films that may have been present on the slices. The polysilicon layers were implanted at room temperature with 5 x 10^{15} cm^{-2}, 40keV arsenic ions (LSS range 0.027 \pm 0.012um). The arsenic was then driven-in at 1000°C in dry oxygen for either 5, 20, or 40 min, producing a surface oxide layer and reducing the thickness of the initial polysilicon layer. For example, after the 40 min drive-in, the surface oxide layer was \( \approx 0.07\mu m \) thick and the initial polysilicon layer was \( \approx 0.10\mu m \) thick. TEM examinations were made with a Philips EM300 operated at 100keV using either plan-view or cross-section specimens. Rutherford backscattering studies were performed with a 1.5MeV helium ion-beam initially aligned along one of the crystal directions in the single-crystal silicon slice (channelled spectrum), and then with the beam misaligned (random spectrum).

2. TEM Results For the polysilicon layers as-deposited onto the silicon slice, TEM plan-view specimens showed that the grains were of mean lateral size 0.05μm (Fig.1a). TEM cross-section specimens revealed that the grains were columnar and extended completely through the 0.14μm thick layer, and that individual layers were reasonably uniform in thickness (Fig.1b). Selected-area transmission electron diffraction patterns indicated that the grains were randomly orientated crystallographically. For the polysilicon layers that had been implanted, cross-section specimens showed that the layers had been converted to amorphous material to a uniform depth of...
\( \approx 0.07 \mu m \) (Fig. 1c). In each of Figs. 1b and c, the lower arrow indicates the silicon slice/polysilicon layer interface, and the upper arrow indicates the polysilicon layer surface.

For the specimens that had been plasma-etched prior to the polysilicon layer deposition, and then given an oxidation drive-in, the results were as follows. For a specimen given a 20 min drive-in, and also a specimen given a 40 min drive-in, all areas of the initial polysilicon layer were polycrystalline (Figs. 2a and b). The mean lateral grain size was 0.15 \( \mu m \), and the grains extended completely through the layer. The grains were randomly orientated crystallographically and were heavily twinned. In Fig. 2b (and also Figs. 3b, 3c, 4b and 4c), the lower arrow indicates the silicon slice/initial polysilicon layer interface (termed interface 1), and the upper arrow indicates the initial polysilicon layer/surface oxide layer interface (termed interface 2).

For a second specimen given a 40 min drive-in, in some areas the initial polysilicon layer was completely polycrystalline as in Fig. 2, while in other areas the layer was partly polycrystalline (P) and partly single crystal (S) (Figs. 3a and b), with the single crystal regions being typically 1 \( \mu m \) across. The areas of this layer that were partly polycrystalline and partly single-crystal showed pronounced local variations in thickness (Fig. 3c). A band of fine damage 5 to 30 \( \mu m \) thick and consisting of small dislocation loops and clusters was present at interface 1 (Fig. 3c). This damage occurred both where the initial polysilicon layer was still polycrystalline and where it had regrown as single crystal.

For the specimens that had been dip-etched prior to the polysilicon layer deposition, the results were as follows. For specimens given either a 20 or 40 min drive-in, all areas of the initial polysilicon layers were single crystal (Figs. 4a and b). The layers contained defects (D), e.g. dislocations, stacking faults and micro-twin lamellae, of density \( \approx 2 \times 10^8 \text{ cm}^{-2} \) (as referred to plan-view specimens) and these threaded completely through the layer. A band of fine damage was present at interface 1 (Fig. 4c). The specimen given a 5 min drive-in was not available for TEM examination.

For the layer of Fig. 4 that was completely single crystal, particular diffraction conditions were used so as to reveal the defects present, and the contrast for the individual stacking faults and micro-twin lamellae was especially pronounced. For the layer of Fig. 3 that was partly polycrystalline and partly single crystal, defects (D) occurred in the single crystal regions similar to those shown in Fig. 4. However, for Fig. 3 different diffraction conditions were used so that these defects were not revealed, this being done so that the distinction between the polycrystalline and single-crystal regions could be more readily made. Different diffraction conditions were mainly also responsible for the different appearances of the surface oxide layer (that arose from the oxidation drive-in) in the various cross-section specimens. Thus, this layer is not readily seen in Fig. 2b, appears grey in Figs. 3b, 4b and 4c, and appears bright in Fig. 3c.

3. RBS Results For the RBS spectra obtained and shown in Fig. 5, the main curves corresponded to backscattering by silicon atoms, but additional peaks arose from backscattering by oxygen and arsenic atoms. For the plasma-etched specimens, the results were as follows. For the specimen given a 20 min drive-in (Fig. 5a), the channelled yield was less than the random yield for energies less than 0.75 \( \text{MeV} \), but was the same for energies between 0.78 and 0.83 \( \text{MeV} \). The former energies corresponded to the silicon slice, and the lower yield was expected because of the channeling occurring in the single-crystal silicon slice. The latter energies corresponded to the initial polysilicon layer, and the same yield indicated that the layer was still completely polycrystalline. The additional peaks were explained as follows. The narrow peak at 0.56 \( \text{MeV} \) corresponded to the oxygen present in the surface oxide layer arising from the oxidation drive-in. The slight shoulder at 0.85 \( \text{MeV} \) corresponded to the silicon present in the surface oxide layer. The separate broad peak at 1.08 to 1.20 \( \text{MeV} \) corresponded to the arsenic present in the surface oxide layer, the initial polysilicon layer and the silicon slice.

For the plasma-etched specimen given a 40 min drive-in that was shown by TEM to possess a partly polycrystalline and partly single-crystal layer, the channelled yield between 0.78 and 0.83 \( \text{MeV} \), which corresponded to the initial polysilicon layer,
showed a pronounced plateau at a height intermediate to that expected for completely polycrystalline material and completely single-crystal material (Fig. 5b). This result indicated that the layer had partly regrown. For this specimen, the silicon in the surface oxide layer gave a shoulder in the random yield at 0.85 MeV as before, but now produced a definite peak in the channelled yield at this position. The second plasma-etched specimen given a 40 min drive-in that was shown by TEM to possess a completely polycrystalline layer was not available for RBS studies.

For the dip-etched specimens, the results were as follows. For the specimen given a 5 min drive-in, the spectra were similar to those of Fig. 5a indicating that the initial polysilicon layer was still completely polycrystalline. For the specimens given either a 20 or 40 min drive-in, the spectra were as in Fig. 5c. The channelled yield between 0.78 and 0.85 MeV, which corresponded to the initial polysilicon layer, was now continuous with the yield from the lower energies, which corresponded to the single-crystal slice. This indicated that the layer had completely regrown.

From the broad peaks of the channelled spectra at 1.08 to 1.20 MeV, total arsenic concentration vs depth curves were deduced and three of these are shown in Fig. 6. These profiles were all of the same general shape with peaks occurring at both interface 1 and interface 2. The shapes depended on the oxidation drive-in times, but not significantly on whether the initial silicon slices had been given a plasma-etch or a dip-etch. The profiles showed that a progressive movement of interface 2 towards interface 1 occurred as the oxidation drive-in time increased from 5 to 20 to 40 min, corresponding to the progressive growth of the surface oxide layer. From the portions of the profiles which corresponded to the silicon slice, approximate values for the depth of the p-n junction below interface 1 were deduced. The profiles showed that for a 5 min drive-in, the arsenic concentration at interface 1 was \( \sim 6.0 \times 10^{20} \text{ cm}^{-3} \) and the junction depth was \( \sim 0.07 \mu \text{m} \). For a 20 min drive-in, the analogous values were \( \sim 3.8 \times 10^{20} \text{ cm}^{-3} \) and \( \sim 0.11 \mu \text{m} \), and for a 40 min drive-in, they were \( \sim 3.0 \times 10^{20} \text{ cm}^{-3} \) and \( \sim 0.18 \mu \text{m} \). A calculated LSS total arsenic concentration profile corresponding to the distribution of the arsenic in the initial polysilicon layer immediately prior to the oxidation drive-in, is also included in Fig. 6.

4. Discussion The TEM and RBS results taken together indicate that the initial polysilicon layers, implanted with arsenic ions, regrow during the subsequent oxidation drive-in as follows. The regrowth occurs in two stages. First, there is a rapid coarsening of the polycrystalline grains. In particular, the grains change from columnar of lateral width 0.05 \( \mu \text{m} \) to equiaxial of lateral width 0.15 \( \mu \text{m} \), the latter dimension corresponding approximately to the polysilicon layer thickness. This behaviour represents the growth of some grains at the expense of others, and is not directly related to the fact that the polysilicon layer was deposited onto a single-crystal silicon slice. (The same grain coarsening behaviour was observed in analogous experiments simultaneously performed but not reported above using similar polysilicon layers that had been deposited onto thick surface oxide layers.)

Second, after the elapse of a certain threshold time, new grains start to form at a number of centres at the initial polysilicon layer/silicon slice interface with the same crystallographic orientation as the silicon slice. These new grains grow upwards and sideways to form small single-crystal regions extending completely through the layer, and these regions eventually join up to produce a complete single crystal layer of the same crystallographic orientation as the silicon slice. For the plasma-etched specimen given a 40 min drive-in which contained both single-crystal and polycrystalline regions (Fig. 3a), the mean spacing between the single-crystal regions was \( \sim 3 \mu \text{m} \) indicating that in this case the number of centres nucleating the new grains at the interface was \( \sim 10^7 \text{ cm}^{-2} \). The crystallographic defects present in the final single-crystal layer probably arose both as the new single-crystal grains grew sideways along the initial polysilicon layer/silicon slice interface, possibly because of interactions with the dislocation loops and clusters present in the narrow band of damage located at this interface, and as the individual new single-crystal regions joined with one another, possibly due to small crystallographic mismatches between them.

The TEM and RBS results show that the threshold time for the plasma-etched specimens is slightly greater than 40 min, but for the dip-etched specimens is between 5 and 20 min. This difference in threshold time was consistently obtained when further specimens were similarly prepared and examined. The reason for this difference is
considered to be as follows. After the silicon slices are plasma- or dip-etched, a thin oxide film remains or is formed on the surface of the slice. When a polysilicon layer is deposited on the slice, this oxide film is trapped at the polysilicon layer/silicon slice interface. During the subsequent oxidation drive-in, the oxide film progressively disperses due to localised diffusion, and eventually small 'holes' begin to form in the film. It is at these 'holes' that the new grains in the polysilicon layer nucleate with the same crystallographic orientation as the underlying silicon slice. The threshold time for nucleation will depend on the initial thickness of the oxide film. The film thickness is considered to be greater for the plasma-etched specimens, and so the threshold time is greater for these specimens. The narrow band of damage located at the polysilicon layer/silicon slice interface which is present following the oxidation drive-in for both the plasma- and dip-etched specimens is thought to arise from this thin oxide film. A separate examination /1/ has now been made of these specimens prior to the oxidation drive-in using the Auger analysis method. The results confirmed that for all of the specimens an oxide film was present at the polysilicon layer/silicon slice interface, and showed that the films ranged in thickness up to ~1.0 nm and were thicker for the plasma-etched specimens.

The total arsenic concentration profiles obtained from the RBS studies show that after an oxidation drive-in of only 5 min, there is a dramatic redistribution of the arsenic. Before oxidation there is an arsenic peak of ~1.7 x 10^21 cm^-3 just below the polysilicon surface. After oxidation for 5 min there are arsenic peaks of 4.0 x 10^20 cm^-3 at the surface oxide layer/initial polysilicon interface (interface 2), and ~6.2 x 10^20 cm^-3 at the initial polysilicon layer/silicon slice interface (interface 1). This arises because of the rapid diffusion of the arsenic along the boundaries of the initial polysilicon grains to the two interfaces. As the oxidation drive-in continues to 20 and then 40 min, the arsenic peaks at the two interfaces progressively decrease, and arsenic diffuses into the underlying silicon slice to give a progressively deeper p-n junction. Our finding that this diffusion behaviour does not depend significantly on whether the specimen was given a plasma- or dip-etch is thought to be mainly due to the initial rapid diffusion of the arsenic to interface 1, before the polysilicon layer regrows, giving a large arsenic peak at this interface. The subsequent layer regrowth behaviour then has little effect on the diffusion of the arsenic into the underlying silicon slice. In addition it is possible that some of the arsenic present interacts with the narrow band of damage located at interface 1. This may cause slower diffusion into the underlying silicon slice than would otherwise occur because it has to 'break away' from the damage.

The TEM results also show that no detectable crystallographic defects had formed in the underlying silicon slices after the specimens had been given oxidation drive-ins. This was the expected result and is one of the reasons for implanting the arsenic into a polysilicon layer rather than directly into the silicon slice, when appreciable crystallographic defects arise following an oxidation drive-in. Our measurements of the electrical characteristics of bipolar transistors have shown that much better performances occur when the transistors are made using polysilicon than when made by the conventional method (Soerowirdjo et al, to be published). However, when fabricating bipolar transistors with polysilicon it is necessary that the presence of surface oxide films on the initial silicon slices and the regrowth behaviour of the polysilicon layers be under strict control or variable device characteristics will occur, and the results of the present work have helped to reveal some of the factors that are important for this to be achieved.

Acknowledgements The authors wish to thank Mrs J E Duffill for useful discussions, the staff of the Microelectronics Fabrication Facility at the University of Southampton for assistance with the slice fabrication, and SERC for supporting the project.

References

/1/ Duffill, J.E., 'Investigation of interfacial oxide thicknesses between silicon and polysilicon', accepted for ESSDERC, Munich, September 1982.
Micrographic TEM

Figs.1a,1b. Silicium polycristallin non implanté, vue du plan et vue de coté.
Fig.1c. Silicium polycristallin implanté, vue de coté.

TEM Micrographs

Figs.1a,1b. Unimplanted polysilicon, plan view and cross-section.
Fig.1c. Implanted polysilicon, cross-section.

Echelle de grandissement = 200nm

Magnification bar = 200nm

Figs.2a,2b. Traitement au plasma, recuit de 40 min (echantillon no. 1), vue du plan et vue de coté.

Figs.2a,2b. Plasma-etched, 40 min drive-in (specimen 1), plan view and cross-section.

Figs.3a,3b. Traitement au plasma, recuit de 40 min (echantillon no. 2), vue du plan et vue de coté.
Fig.3c. Même chose que Fig.3b, fort grandissement, vue de coté.

Figs.3a,3b. Plasma-etched, 40 min drive-in (specimen 2), plan view and cross-section.
Fig.3c. As 3b, high magnification cross-section.
Figs. 4a, 4b. Traitement chimique, recuit de 40 min, vue du plan et vue de coté.
Fig. 4c. Même chose que Fig. 4b, fort grandissement, vue de coté.

Figs. 4a, 4b. Dip-etched, 40 min drive-in, plan view and cross-section.
Fig. 4c. As 4b, high magnification cross-section.

Spectres RBS
Fig. 5a. Traitement au plasma, recuit de 20 min.
Fig. 5b. Traitement au plasma, recuit de 40 min (échantillon no. 2).
Fig. 5c. Traitement chimique, recuit de 40 min.

RBS Spectra
Fig. 5a. Plasma-etched, 20 min drive-in.
Fig. 5b. Plasma-etched, 40 min drive-in.
Fig. 5c. Dip-etched, 40 min drive-in.

Profils d'arsenic
Fig. 6a. Implanté, LSS.
Fig. 6b. Traitement chimique recuit de 5 min.
Fig. 6c. Traitement au plasma, recuit de 20 min.
Fig. 6d. Traitement chimique, recuit de 40 min.

Arsenic Profiles
Fig. 6a. As-implanted, LSS.
Fig. 6b. Dip-etched, 5 min drive-in.
Fig. 6c. Plasma-etched, 20 min drive-in.
Fig. 6d. Dip-etched, 40 min drive-in.