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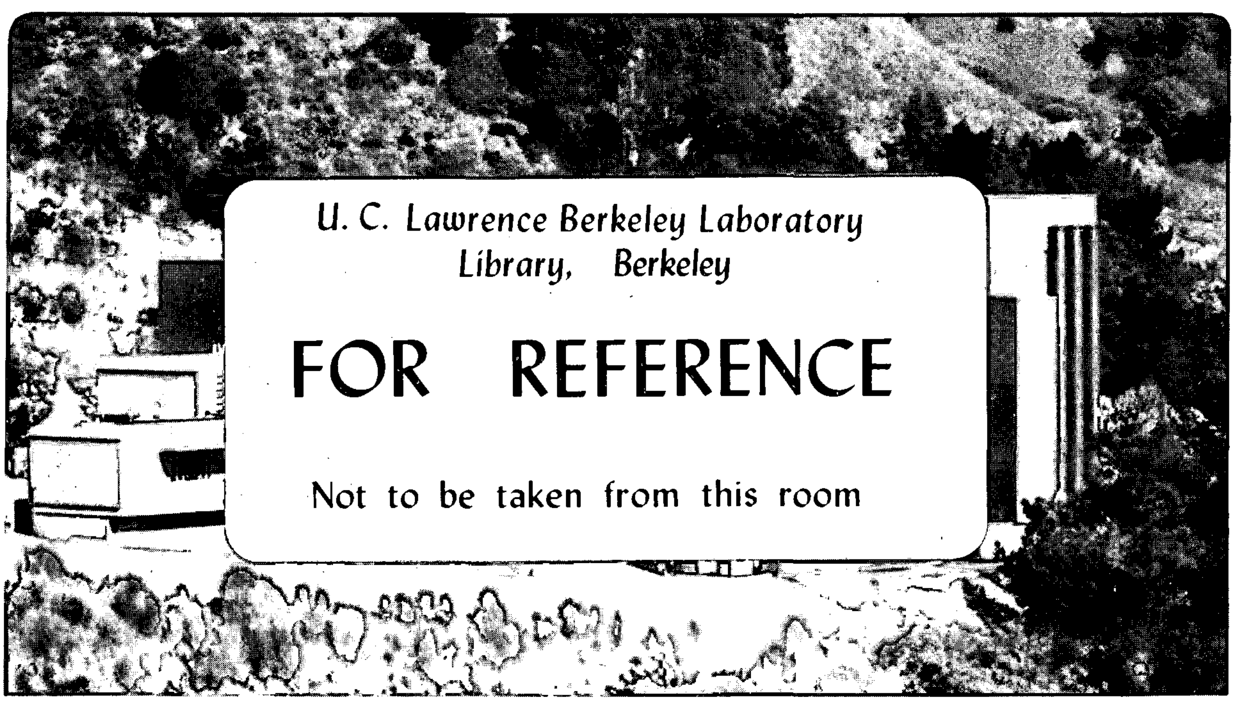

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SOI Interface Structures in Selective Epitaxial Growth

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ABSTRACT

Silicon-on-insulator structures were formed by the selective epitaxial growth (SEG) of silicon and the epitaxial lateral overgrowth (ELO) of oxide shapes using an LPCVD hot-walled reactor at 850°C. The homoepitaxial interface changed character with modifications of the gas composition during the in-situ pre-epitaxial bake at 900°C. HREM images show ellipsoid-shaped inclusions lying along the homoepitaxial interface for silicon growth conducted with no dichlorosilane (DCS) flow during the prebake in H_2. SIMS analysis indicates a large oxygen, fluorine, and carbon concentration at the interface. For structures grown with a small DCS flow in addition to H_2 during the prebake, the homoepitaxial structural defects and the oxygen, fluorine, and carbon peaks are removed.

INTRODUCTION

In the interest of obtaining increased integrated circuit device density, a relatively new technology known as selective epitaxial growth (SEG) of silicon is being explored, especially for improved isolation of devices including possible three dimensional (vertical) integration of devices.[1-3] This technology involves the deposition and selective nucleation and growth of silicon from the vapor phase, seeded by the silicon substrate. The process is "selective" because nucleation and growth occurs on the silicon substrate but is prohibited on the oxide. The epitaxial silicon proceeds to grow upward and over the oxide laterally. The interfaces created by this process (figure 1) require detailed structural analysis, as the quality of these structures affect the electrical properties of the devices.

The presence of residual non-silicon phases at the silicon substrate surfaces (such as SiO_2 or Si-C complexes) can destroy the quality of the homoepitaxial interface. Removal of "native oxide" is critical. It has been demonstrated that an increased temperature [4] and a reduction of oxygen and water content [5] in the furnace environment can cause silicon dioxide decomposition in the form of SiO(g). In an attempt to reduce oxygen and water content, a small amount of dichlorosilane gas is added to the prebake cycle.[6] As discussed elsewhere, the addition of DCS is beneficial; the density of homoepitaxial inclusions is greatly reduced. [6]

Most of the published literature focuses on characterizing the macroscopic structural qualities of the silicon epilayers as determined by using optical microscopy.[7,8] However, by using conventional and high resolution transmission electron microscopy we can determine the degree of structural perfection of these silicon-on-insulator structures. In this paper, we present the results of a transmission electron microscopy study of the homoepitaxial interface (interface #1) and examine the effects of the prebake environment on this interface.

EXPERIMENTAL PROCEDURE

Silicon deposition was performed in a hot-walled low pressure chemical vapor deposition (LPCVD) reactor.[6] Four-inch p-type silicon wafers with a resistivity between 30 to 50 ohm-cm were used as the substrates. The silicon wafers were prepared using a standard cleaning procedure. A thermal oxide was then grown at 1000 °C. Conventional lithography was performed such that the oxide sidewalls were aligned towards the <100> direction rather than the standard <110> direction. Windows in the oxide were etched using plasma etching. A 25 nm sacrificial oxide was then grown at 900 °C and removed using a dilute HF solution. Pre-epitaxial cleaning included two H_2SO_4-H_2O_2 (Pirahna) treatments with an intermediate dilute HF dip to remove any oxide grown during cleaning. An additional HF vapor exposure (1:2 H_2O:49% HF) was performed for 5 seconds immediately before loading.

A prebake was performed at 900 °C with a pressure of 6 torr in an H_2 ambient. Silicon deposition was performed at 850 °C at a pressure of 0.6 torr. In some cases, a small concentration of DCS was added during the prebake (0.025%). Secondary ion mass spectrometry (SIMS) was performed at Charles Evans Inc.

Cross-sectional transmission electron microscopy specimens were prepared using conventional techniques. After mechanical thinning to about 30 μm, specimens were ion milled to a thickness suitable for electron transparency. Electron microscopy was performed on the JEOL 200 CX operating at 200 kV at the National Center for Electron Microscopy. The SOI interfaces formed by epitaxial lateral overgrowth of oxide shapes is shown in figure 1. All micrographs were taken in the [011] zone axis.

RESULTS

In figure 2, a conventional TEM image of the homoepitaxial interface grown with no DCS flow during the prebake shows inclusions along the (001) homoepitaxial interface. These defects lie discontinuously along the interface. SIMS analysis in figure 3 shows a sharp increase in oxygen, fluorine, and carbon content at the homoepitaxial interface.

At the edge of the homoepitaxial inclusion, a HREM image in figure 4 reveals an ellipsoidal shape, ending at a region of perfect homoepitaxy. The lattice planes are continuous across the homoepitaxial interface, even across the inclusion area, indicating that these defects are not isolated dislocation cores.

A HREM image of an edge of a different (001) inclusion is presented in figure 5. The height of this defect region extends for about 10 monolayers normal to the homoepitaxial interface. Similar to the interface shown in figure 4, there still exists a region of perfect homoepitaxy and no discontinuities of the lattice planes throughout the homoepitaxial interface. Within the defective region, there are three rows of clearly visible lattice planes surrounded by an envelope of darker contrast, the origin of which is believed to be strain-related.

In figure 6, a conventional TEM image of an SOI structure grown with DCS flow during the prebake indicates no inclusions along the homoepitaxial interface. SIMS analysis in figure 7 reveals no oxygen or fluorine peaks at the interface.

DISCUSSION

Since the presence of the ellipsoidal defects lying along the (001) direction are related to the presence of oxygen (and possibly fluorine and carbon) at the homoepitaxial interface, the formation of these ellipsoidal defects might be caused by the entrapment of

SiO_2 or other phases during silicon growth before decomposition is complete. Rubloff [4] has demonstrated for example, that SiO_2 decomposition occurs through the reaction

$$Si(s) + SiO_2(s) \rightarrow SiO_2(g).$$

Decomposition begins with void formation in the SiO_2 film and proceeds with the growth of these voids. If silicon deposition begins before all SiO_2 is removed from the homoepitaxial interface, ellipsoidal defects of the types shown in figures 4 and 5 can be formed. Once some SiO_2 decomposition has occurred but not complete, regions exhibiting perfect homoepitaxy will be present among the ellipsoidal defects. These ellipsoidal defects have been previously observed in silicon homoepitaxy using MBE.[9]

The continuity of the lattice planes through the epitaxial film, as shown in figures 4 and 5, is not disturbed even with the presence of the ellipsoid defects; one might therefore infer that the lateral overgrowth of the ellipsoid defects occurs in a similar manner to the lateral overgrowth of oxide shapes. The epitaxial silicon must grow "up and over" the ellipsoid defect, implying growth selectivity of silicon sites over these oxygen/carbon/fluorine ellipsoid defects. If the deposition of silicon were not selective over the ellipsoid defects, polysilicon nuclei could be formed on the ellipsoid defects and result in great discontinuity of structure in the epitaxial film over the defective regions.

As the addition of DCS during the prebake cycle eliminates the ellipsoid defects, it is apparent that the addition of DCS does enhance SiO_2 decomposition. DCS may decrease the partial pressures of oxidants in the furnace by precipitation reactions, for example:

$$SiH_2Cl_2(g) + 2H_2O \rightarrow SiO_2(s) + 2HCl(g) + H_2(g).$$

This reaction could occur upstream from the wafers and the resulting $SiO_2(s)$ is either deposited or blown out by a high flow rate of hydrogen.

Although a structurally "perfect" homoepitaxial interface exists, the question of the exact location of the epitaxial silicon/ silicon substrate homoepitaxial interface still remains. Using scanning tunneling microscopy (STM), Sun [10] has shown that the decomposition of $SiO_2(s)$ into $SiO(g)$ can effectively roughen the silicon substrate surface between 4 to 10 monolayers. Thus, the homoepitaxial interface does not lie in a straight line, but follows a rough path traversing several silicon substrate monolayers. This may explain the variation of the location of the ellipsoidal defects as seen in figure 2. From the Kossel model of epitaxial growth where adatoms prefer to settle in kink sites over step sites, the roughening of the silicon substrate may facilitate homoepitaxial growth.

SUMMARY

An effect of dichlorosilane flow during the prebake cycle on epitaxial lateral overgrown silicon-on-insulator structures has been investigated using HREM. Without DCS in the prebake cycle, ellipsoid shaped inclusions were found at the homoepitaxial interface. SIMS analysis suggests that these defects contain oxygen, fluorine, and carbon. The addition of DCS to the prebake cycle was effective in removing the inclusions by aiding the decomposition of non-silicon phases on the silicon substrate surface. A perfect homoepitaxial interface resulted.

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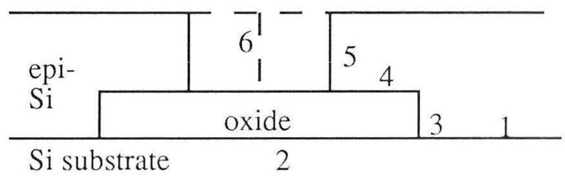

XBL 921-133

Interfaces:

1. Homoepitaxial
2. Thermal SiO2/ Si
3. Oxide Sidewall
4. Epi Si/ SiO2
5. Epi Si growth front
6. Intersection of Growth Fronts

Figure 1: Interfaces Created by Epitaxial Lateral Overgrowth

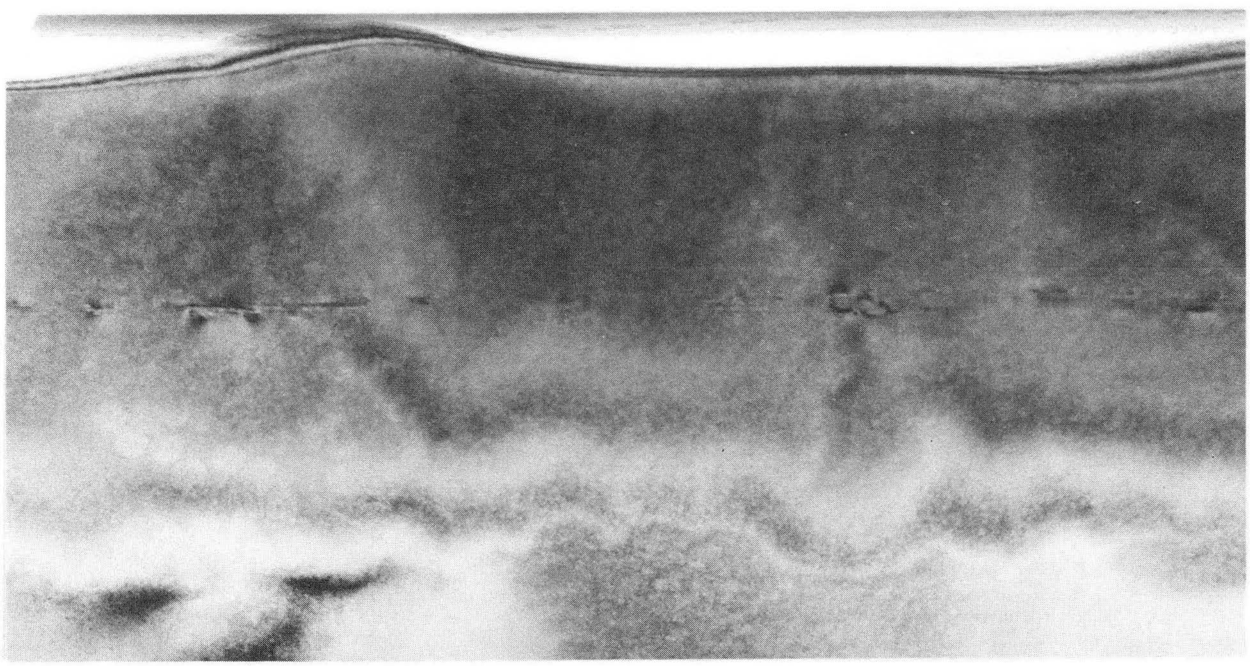

Figure 2: Conventional TEM Image of Homoepitaxial Interface grown with no DCS flow during prebake

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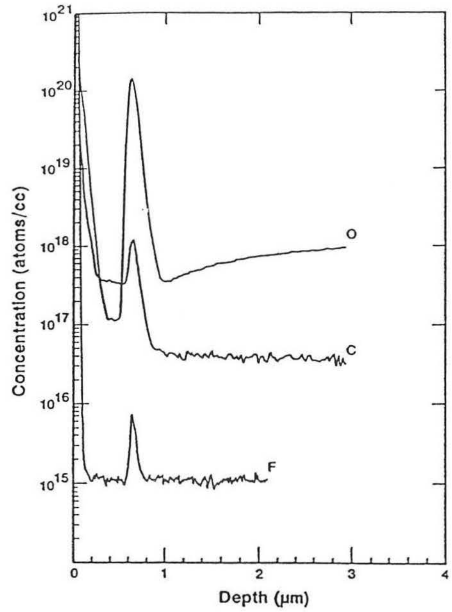

Figure 3: SIMS Profile of Epi Film grown with no DCS flow in prebake XBL 921-135

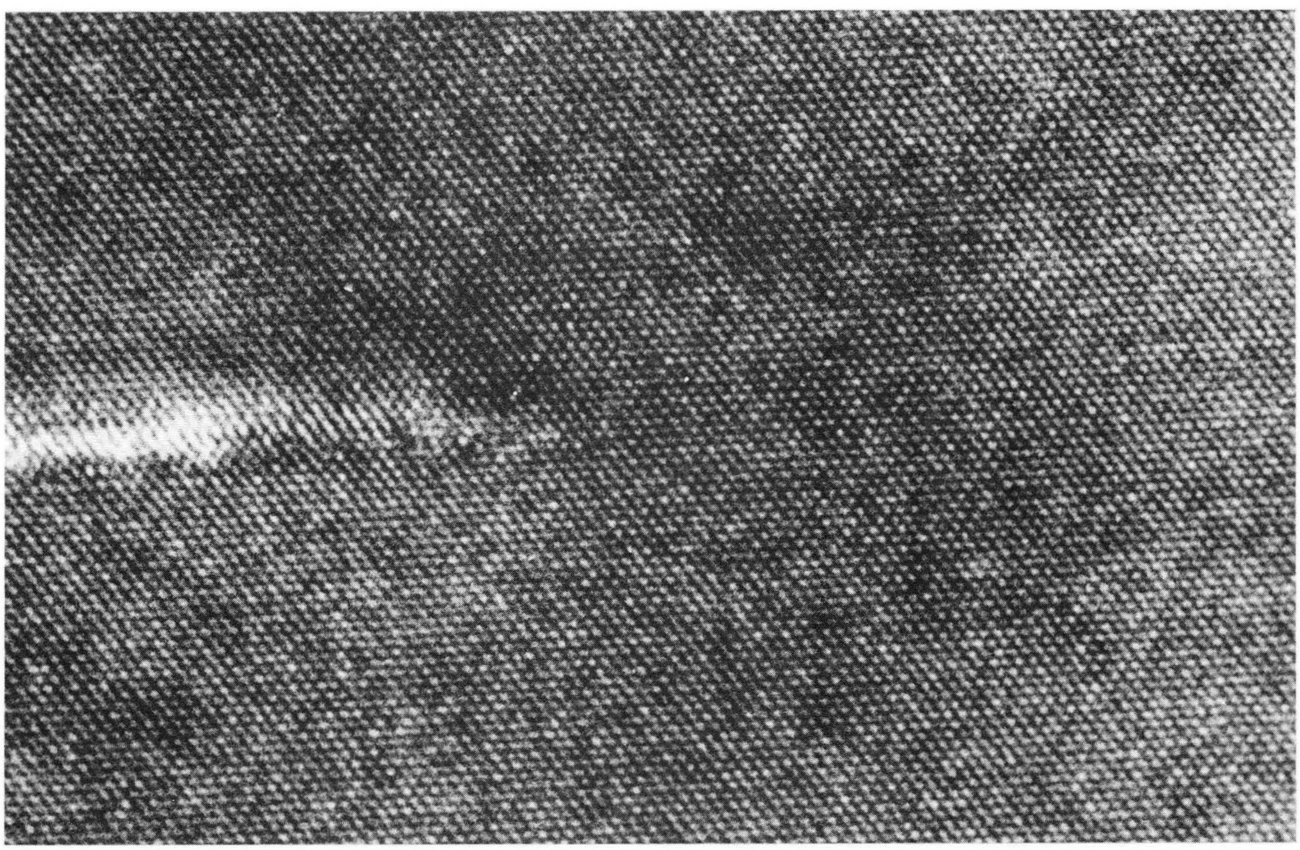

Figure 4: HREM Image of Homoepitaxial Interface (no DCS flow in prebake) XBB 9112-9775

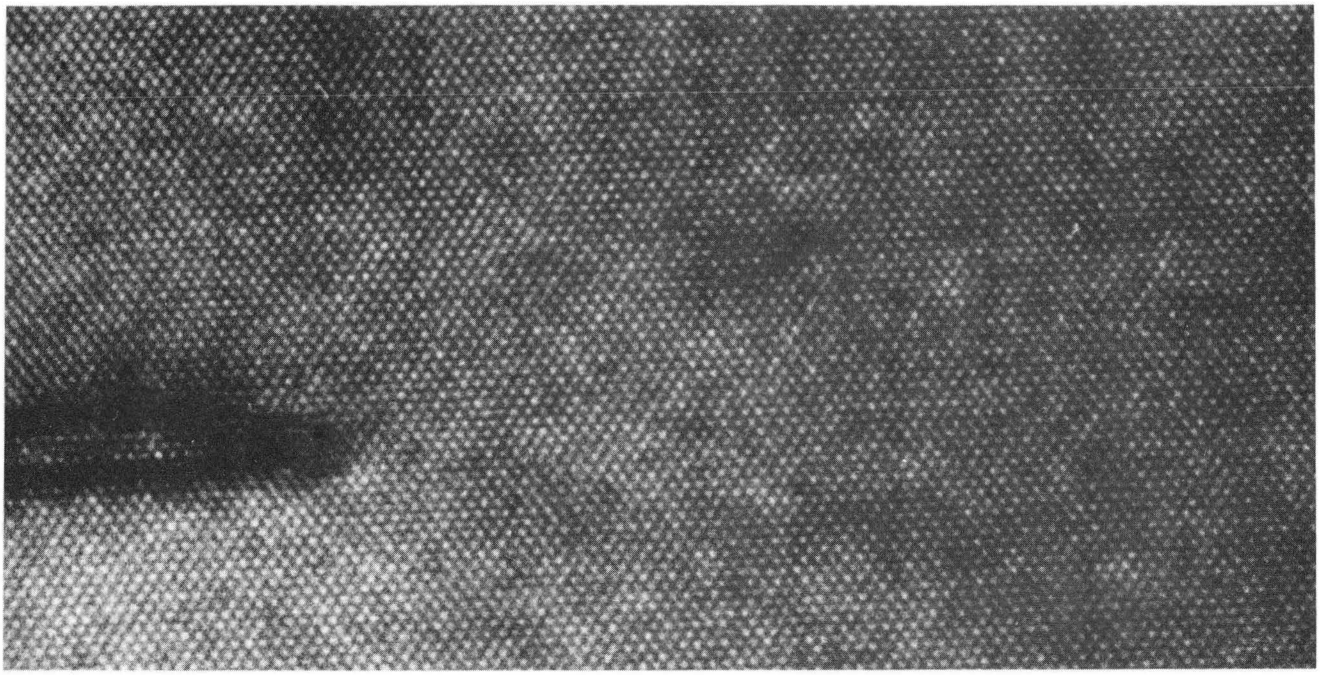

Figure 5: HREM Image of Homoepitaxial Interface (no DCS flow in prebake) XBB 9112-9774

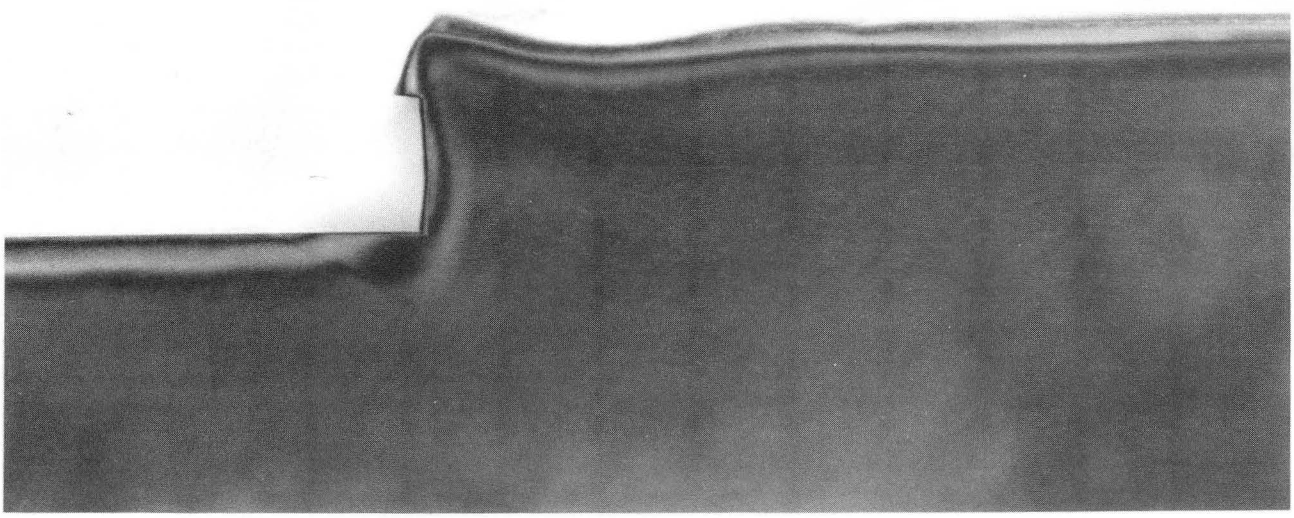

Figure 6: Conventional TEM Image of Homoepitaxial Interface grown with DCS flow during prebake XBB 921-191

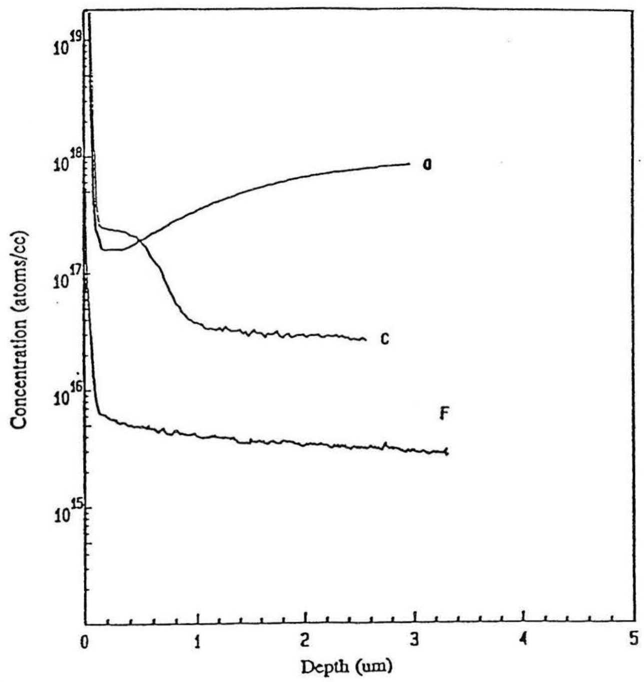

Figure 7: SIMS Profile of Epi Film grown with DCS flow in prebake

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