

**Bonded Silicon Silicide on Insulator (S²OI)
A Study of Chemical, Physical and Optical Properties
for Advanced Device Fabrication**

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ABSTRACT

Bonded silicon silicide on insulator materials (S²OI) are a recent introduction into the commercial market place. For their full acceptance into device manufacturing lines the properties and behaviour of these materials must be well understood. This study reports some of the physical/optical properties and the impurity behaviour of S²OI structures. The formation of large grains of buried silicide and their impact is reported. Also, the diffusion of dopants adjacent to the silicide and SIMS contamination studies of the SOI layer are discussed. Early Surface Photo-Voltage (SPV) results indicate that buried silicide wafers do not lead to the contamination of adjacent bulk wafers in high temperature furnaces. These studies indicate that S²OI substrates are suitable for device manufacture.

INTRODUCTION

The availability of Silicon On Insulator (SOI) materials with highly conducting buried silicide layers offers new device opportunities in both the optical and electronic fields. Optical characterisation of the silicon-silicide interface is important for devices such as photo-detectors as well as for optical characterisation tools (ellipsometers and reflectometers) which would be used for measuring SOI parameters [1] during device processing. Electronic and structural characterisation includes sheet resistance, morphology, stress, crystalline quality of the overlying Si layer, contamination of the overlying layer and any diffusion anomalies caused by the buried silicide layer.

In this paper, we present an optical model for the tungsten silicide silicon interface based on the morphology of the silicide-silicon interface and the newly measured optical properties for the buried silicide. We show that the buried silicide, which has high conductivity, results in low stress in the overlying silicon and is free of heavy metal contamination (to SIMS sensitivity) or crystal damage. Furthermore, we show that this buried silicide layer has no anomalous effect on the out diffusion of standard silicon dopants.

EXPERIMENTAL

Sample Preparation. Physical and Optical Studies

The formation of the buried silicide structures has been described elsewhere [2,3]. The optical (complex refractive index, n and k) and interfacial properties of the buried silicide were investigated by spectroscopic ellipsometry (SE), atomic force microscopy (AFM) and cross-sectional TEM. The n and k constants, of the buried silicide, were measured by SE after either selective wet chemical etching or by chemomechanical polishing down to the silicide layer of the overlying Si layer. In addition SIMOX wafers [4] were coated with a silicide and bonded. Using the buried oxide as a etch stop layer, S2OI structures in which the silicide was actually thicker than the top silicon film were formed. This allowed the optical characterisation of a thin known silicon thickness S2OI structure to verify the values obtained on the conventionally thinned samples. The optical properties of as-deposited silicide films were also measured as a reference.

The n and k values were determined by direct inversion of the ellipsometric parameters for the deposited, etched and polished silicide materials. The buried silicides were quite different from the as-deposited amorphous material due to poly- crystalline grain growth during the thermal bonding cycle. Si-like structure in the n and k data just below 300nm and at about 350nm confirms this (figure 1). As-deposited silicides do not display the crystalline optical transitions. -This grain growth results in a higher Si/silicide interfacial roughness, much greater than the roughness of the amorphous-like as-deposited silicide. Figure 2 shows a cross-sectional TEM of the buried silicide, overlying silicon and buried oxide. The uniformity of the silicide was good with large single grains traversing the whole film thickness. The back oxide interface was smoother than to the overlying silicon layer. This is because the silicon is more likely to react with the silicide than the oxide and it is well known that the mobile species in silicides is Si. AFM measurement of the RMS roughness (from the PSD within the bandwidth of 15nm to 3000nm) of the as-deposited silicide is about 2 nm (RMS). This is increased to around 17 nm (RMS) for the bonded wet etched silicide surface, while the polished silicide is again around 2 nm (RMS). AFM images of the etched sample show

the granularity of the silicide film clearly. Indeed the wet etched material can be modelled using the optical functions of the smooth polished silicide sample combined with a surface roughness layer (a mixture of silicide and void) of $15.1 \pm 0.7\text{nm}$. This is very close to the RMS roughness measured for the wet etched sample from AFM.

This new optical data has been used to model complete S²OI structures. Figure 3 shows the experimental spectroscopic ellipsometric (SE) data and the fitted model from the buried silicide bonded SIMOX SOI. The value (-240nm) calculated for the silicon layer is essentially the same as the starting SIMOX wafer. The interfacial layer was calculated to be $159 \pm 6\text{\AA}$, which is close to the roughness layer thickness determined above. A more detailed discussion of the optical properties and interfacial roughness can be found in Thin Solid Films (in press).

An important aspect to note is that detailed interfacial inspection with both SEM and TEM over long distances (mms for SEM and 10s of ums for TEM) of the interface did not reveal the presence of any voids on either the silicon side or the oxide side. This indicates that the interfaces are stable after the thermal bonding cycle. Strain contours are present in the silicide grains and the large roughness and sharp interface between the silicide and silicon result in a strong strain field in the silicon extending to about 200nm. A much weaker strain field can be seen extending to at least one micron into the silicon suggesting gettering potential for this film.

SIMS Analysis for Chemical Constituents and Impurity Species.

Impurities play an important part in the behaviour of electronic devices. We have analysed both the potential out diffusion of tungsten from the silicide layer as well as out diffusion of common dopants. Tungsten silicide is a commonly used material - in IC processing without reported heavy metal contamination of the bulk silicon layer . However, because of the unique construction on this wafer and the higher temperatures involved, it is important to re-confirm this. SIMS analysis using both O and Cs of the S²OI structures revealed an abrupt W profile at the silicide/Si interface (figure 4). This strongly confirms that the W does not diffuse into the Si and remains confined to the silicide. The as-deposited silicide is Si rich and hence limits the motion of W. An important aspect to note is that metallic impurities were also profiled and found to be below the SIMS sensitivity levels for the bulk of the single crystal SOI layer, for both undoped silicides and doped silicides (which were ion implanted prior to bonding). Low levels, just above the SIMS sensitivity limits, of some metallic impurities were found only immediately adjacent to the silicide layer. This may be the result of changes in ion yields near the silicide layer .

As previously reported [2] undoped silicides on N-type wafers *form* Schottky barriers at the Si/silicide interface. However, n-type doping introduced by ion implantation (e.g. As -101Jcm⁻²) prior to bond leads to ohmic electrical behaviour. Ohmic behaviour was found for P-type material with or without an implantation. Therefore, it is important to understand the diffusion of common species into the silicon SOI layer using the doped silicide as a source. This is not only important for ohmic contact formation but for doped well formation as well. Because the silicide is refractory, it is possible to implant it and use it as a diffusion source to *form* a deep lightly doped well profile which can be useful for many applications.

As a result, silicided wafers were implanted with various doses of arsenic, phosphorous, or boron prior to bonding. These wafers were then bonded at 1050°C (60 minutes) and annealed sequentially at 1150°C (45 minutes) and 1000°C (7 hours). In all cases, the outdiffusions showed no anomalous effects and diffused similarly to implants into control wafers without silicide. Figure 5 shows an example of a Ph doped (5×10^{14} cm⁻² at 170KeV) wafer. The SIMS profile and the Suprem 3 simulation show good agreement indicating that the silicide interface is not a source of defects causing enhanced diffusion nor does the silicide or the silicide-silicon interface trap dopants or inhibit their diffusion. These results confirm the TEM results previously which show no voiding and low interfacial stress.

SPV measurements were also taken from bulk wafers processed simultaneously with S²O1 wafers at high temperatures (1150°C dry oxidation for 45 minutes). The diffusion lengths for wafers adjacent to the S²O1 wafers were (139µm and 171µm) comparable to a third wafer (191µm) separated by several wafer boats and within the accepted variability of the test. These results suggest that the buried -silicide does not lead to additional surface contamination during thermal cycles. Further detailed studies are required to confirm these results.

CONCLUSION

Optical, physical and chemical properties of S²O1 materials were studied. The buried silicide layer was found to have significantly changed due to the bonding thermal anneal as revealed by both its optical and structural properties. The important observation that the W was confined to the silicide layer bodes well for electronic devices. Other metallic impurities were also found to be at SIMS sensitivity levels. Well controlled doping layers adjacent to the silicide result in good ohmic behaviour at the silicide/Si interface. Our results suggest that S²O1 materials are a good candidate for many electronic and optical devices.

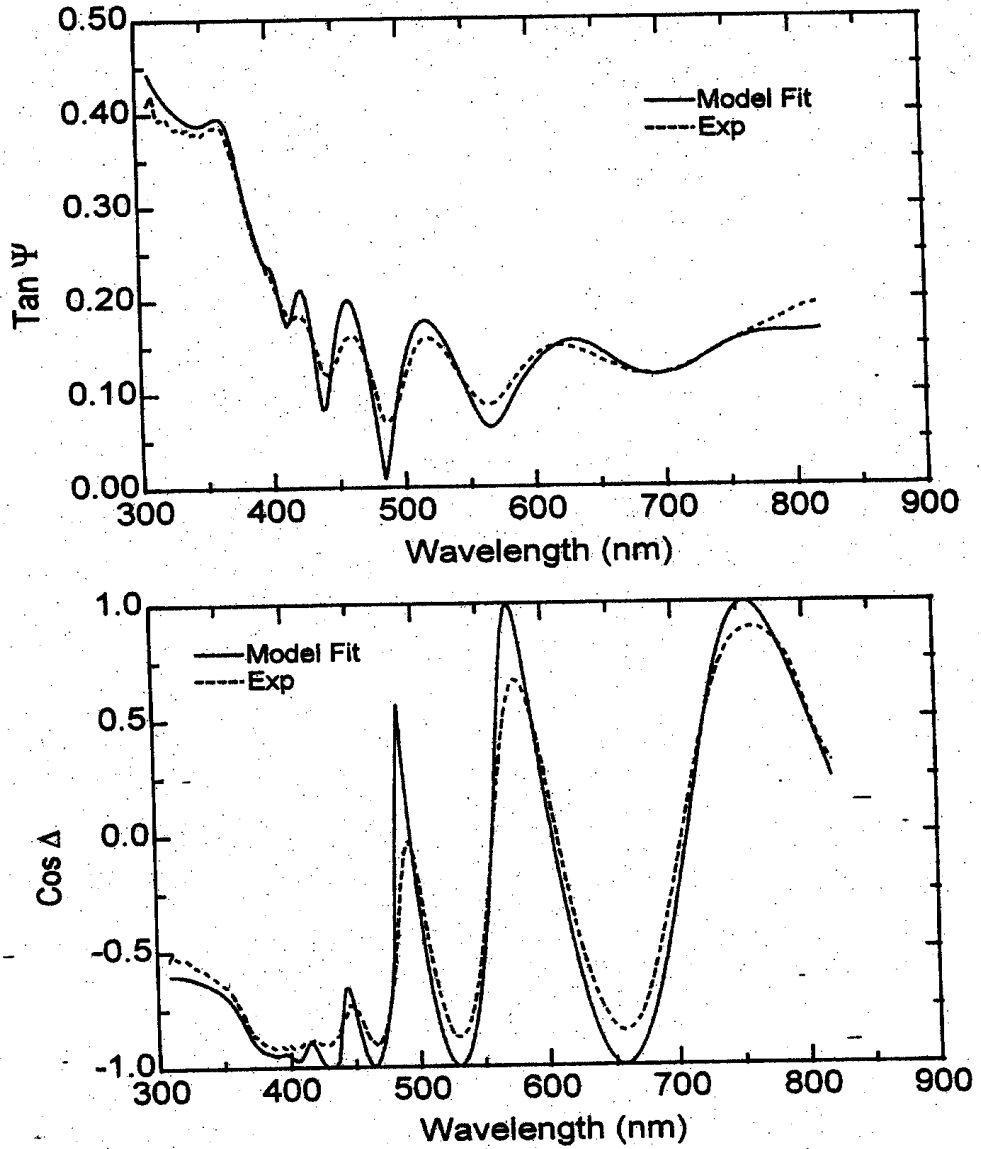


Figure 3 $\tan \Psi$ and $\cos \Delta$ fits for a thin S^2OI sample, yielding a structure consisting of 2 nm surface native oxide, 239.4 ± 1.7 nm of Si, 15.9 ± 0.6 nm interfacial roughness layer (with a 0.4 ± 0.07 fraction of Si mixed with silicide) and the underlying silicide.

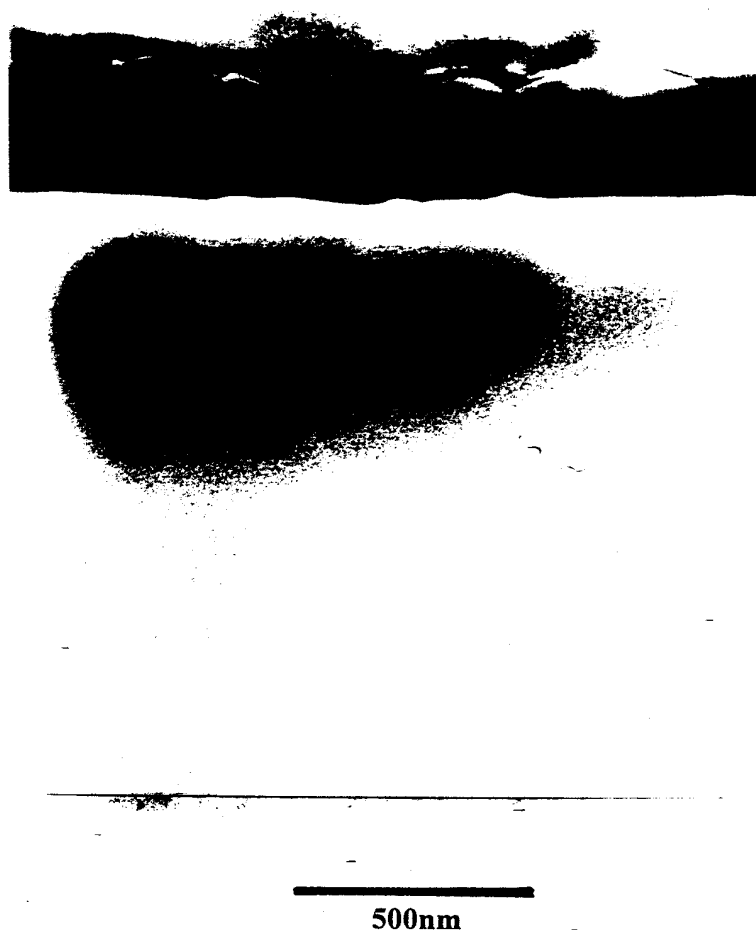


Figure 2 Cross-sectional TEM of S²OI structure showing recrystallised buried silicide. Note strain contours apparent in silicide grains but much weaker strain contour in adjacent silicon.

References

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This work was partly funded by the UK Dept. of Trade and Industry.

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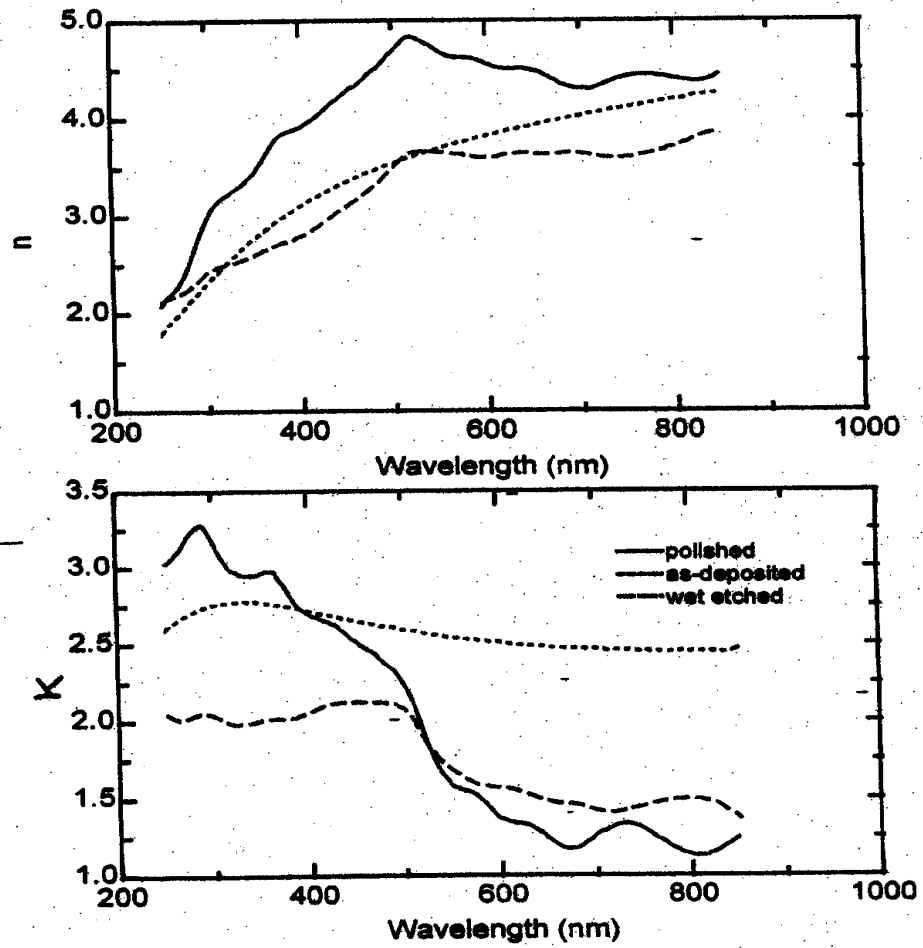


Figure 1 Optical constants of as-deposited, wet etched and polished tungsten silicide layers.

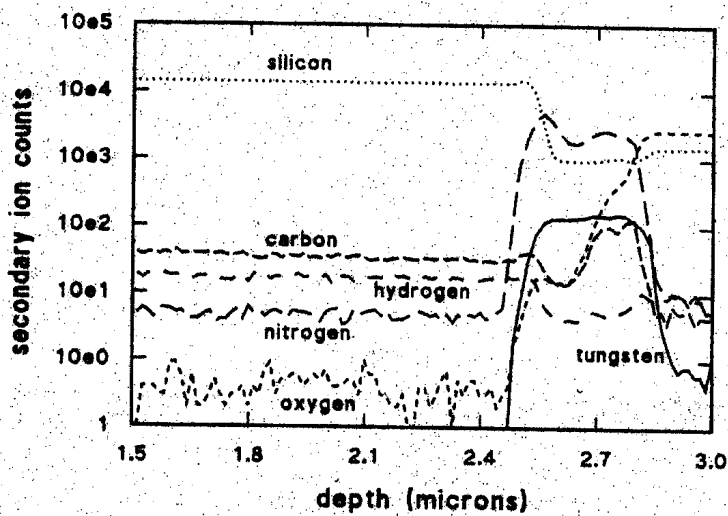


Figure 4 SIMS profile showing the well confined W to the silicide layer and background levels of non-metallic impurities in the bulk of the Si layer.

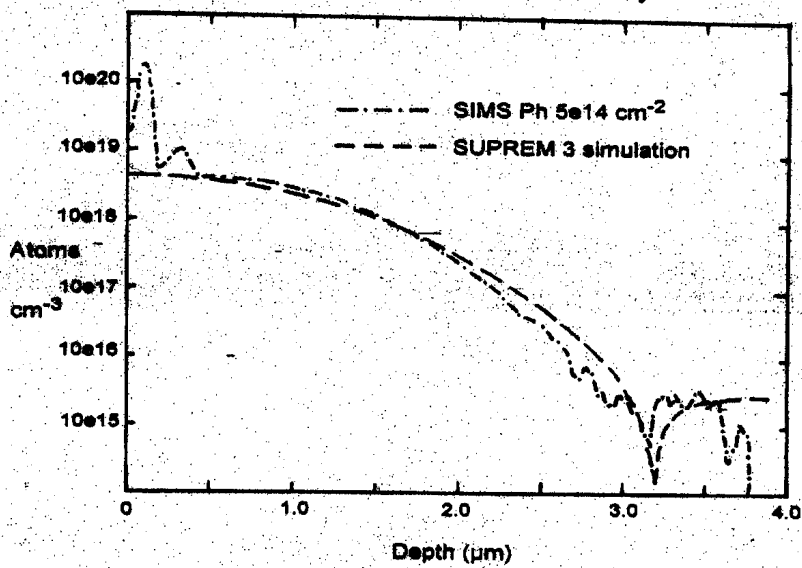


Figure 5 A comparison of SIMS profile and SUPREM 3 simulation of Ph diffusion (see text for thermal cycle).