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# The high growth rate of epitaxial silicon–carbon alloys by using chemical vapour deposition and neopentasilane

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## Abstract

The growth of epitaxy of silicon–carbon ($Si_{1-y}C_y$) alloy layers on (1 0 0) silicon substrates by chemical vapour deposition (CVD) with a novel precursor, neopentasilane, as the silicon source gas and methylsilane as the carbon source is reported. High quality $Si_{1-y}C_y$ alloy layers at growth rates of 18 nm min$^{-1}$ and 13 nm min$^{-1}$ for fully substitutional carbon levels of 1.8% and 2.1%, respectively, were achieved. The highest substitutional carbon level achieved was 2.6% (strained perpendicular lattice constant of 5.347 Å) as determined by x-ray diffraction.

(Some figures in this article are in colour only in the electronic version)

## Introduction

The growth of epitaxial strained silicon–carbon ($Si_{1-y}C_y$) alloys on Si (1 0 0) substrates is of great interest for use in the source–drain regions of MOSFETs. The $Si_{1-y}C_y$ alloys induce tensile strain in channel regions to enhance electron carrier mobility [1]. In this work, the growth of epitaxial $Si_{1-y}C_y$ alloys by chemical vapour deposition with high substitutional carbon fractions ($y \sim 2.6\%$) and extremely high growth rates at 575 °C (~20 nm min$^{-1}$ at $y = 1.8\%$) is reported. The high growth rates are enabled by neopentasilane (NPS), a novel high-order silane silicon precursor.

## Growth of $Si_{1-y}C_y$ alloys layers

High substitutional carbon fraction in $Si_{1-y}C_y$ alloys is important to achieve significant strain for electron mobility improvement. It is difficult to achieve high substitutional carbon percentages in silicon due to the low solubility of carbon in silicon. Non-equilibrium growth techniques such as molecular beam epitaxy (MBE) and chemical vapour deposition (CVD) are used to incorporate a high metastable substitutional carbon fraction [2, 3]. Furthermore, it has been demonstrated that a high growth rate at low temperature favours the incorporation of carbon into substitutional sites [2, 4]. However, achieving a high rate in chemical vapour deposition (CVD) at low growth temperature is difficult.

It is well known that increasing the order of the silane increases the silicon growth rate in chemical vapour deposition. The silicon growth rate using trisilane is higher than that with disilane, which in turn is higher than that with silane. We recently have investigated silicon epitaxial CVD at low temperatures using neopentasilane $Si_5H_{12}$ (figure 1), a novel high-order silane as a silicon source.

Neopentasilane (NPS) $Si_5H_{12}$ is a liquid at room temperature. Hydrogen is bubbled through the liquid to provide a gas source of neopentasilane. The exact neopentasilane flow is not known but estimated at 0.1% of the bubbler flow. Ultra-high growth rates with excellent quality epitaxy have been achieved with this novel precursor [5]. High-resolution cross-section transmission electron microscopy showed no stacking faults, interface defects, or other features, and showed sharp diffraction patterns.

Most of the experiments using NPS were done at a pressure of 6 Torr of hydrogen, and ~0.5 mTorr for the NPS (solid squares). At 600 °C one experiment was done at 6 Torr of hydrogen, and ~2 mTorr for the NPS (open square). At 600 °C, the highest growth rate obtained with NPS (130 nm min$^{-1}$) represents an increase of 3×, 8× and 72× versus the growth rate reported using trisilane, disilane and silane, respectively [6, 7] (figure 2).

The ability to grow epitaxy at ultra-high growth rates at low temperatures makes NPS a promising candidate

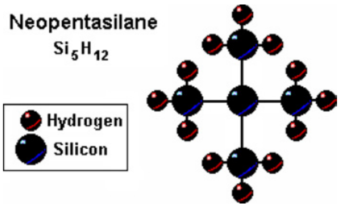

**Figure 1.** Chemical configuration of neopentasilane (NPS).

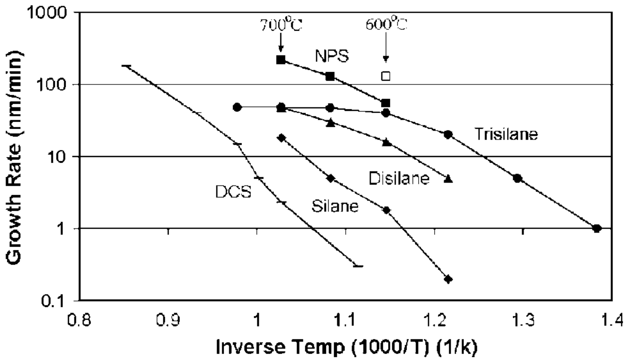

**Figure 2.** Comparison of low-pressure chemical vapour deposition (LPCVD) epitaxial growth rates versus inverse temperature for sources of dichlorosilane (DCS), silane, dislane, trisilane [6, 7] and novel neopentasilane (NPS) precursor on (1 0 0) silicon substrates.

for the growth of $Si_{1-y}C_y$ layers with high substitutional carbon percentages. $Si_{1-y}C_y$ alloys layers were grown pseudomorphically on silicon (1 0 0) substrates by using methylsilane ($SiCH_6$) as a carbon source.

## Characterization

High-resolution x-ray diffraction (HR-XRD) was done to determine the substitutional concentration of carbon in silicon, and SIMS measurements were used for total carbon concentration. In figure 3, a comparison between experiment and simulation for x-ray diffraction of a $Si_{1-y}C_y$ alloy grown with NPS and methylsilane is plotted. The correspondence between experiment and simulation and clear interference fringes indicate a high quality crystalline structure.

The substitutional carbon percentage was calculated from the shift in perpendicular lattice constant $a_\perp$, from that of the substrate. Since the alloy layer grown is in tensile strain, Poisson's ratio is used to convert from the strained lattice constant to the relaxed lattice constant using the following equation [8, 9]:

$$a_{\perp,\mathrm{Si}_{1-y}C_y,\mathrm{strained}} = a_{\mathrm{Si}_{1-y}C_y,\mathrm{relaxed}} + \frac{2c_{12}}{c_{11}} \times \left(a_{\mathrm{Si}_{1-y}\mathrm{C}_y,\mathrm{relaxed}} - a_{\mathrm{Si}}\right). \qquad (1)$$

Various authors calculate the carbon percentage from the perpendicular lattice constant using different techniques, such as applying Vegard's law between silicon and diamond or silicon and silicon-carbide, or by some other method such as that of Kelires [10]. In our case we apply Vegard's law between silicon and diamond for the relaxed lattice constant. Note the effect of strain on the relaxed lattice constant is important. Omission of this effect (the last term in equation (1)) leads one to overestimate the substitutional carbon percentage by a factor of ~1.8.

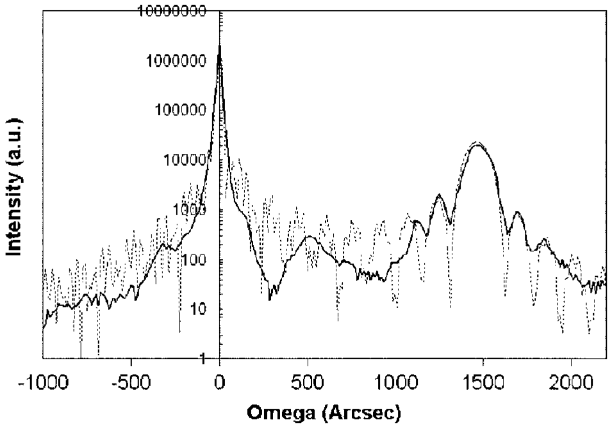

**Figure 3.** High-resolution x-ray diffraction (HR-XRD) of a 130 nm $Si_{1-y}C_y$ layer on Si showing a substitutional carbon level of 1.8% with a lattice constant of 5.375 Å. The solid line represents the raw data while the dotted lines indicate simulation. The growth temperature was 575 °C and the growth rate was 20 nm min$^{-1}$.

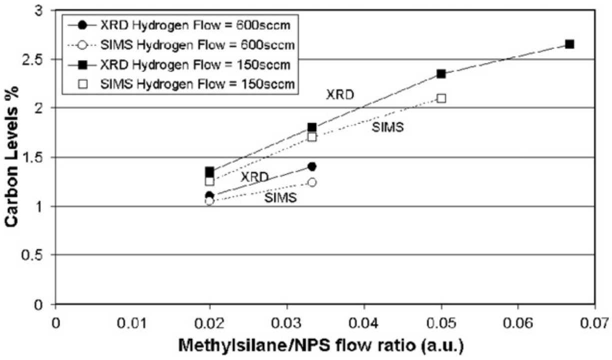

**Figure 4.** Carbon percentage determined by SIMS and calculated from XRD data versus the ratio of methylsilane to NPS source flow at fixed hydrogen flow. The squares represent hydrogen flow of 150 sccm and circles represent hydrogen flow of 600 sccm.

To incorporate a high substitutional carbon percentage in silicon, a high growth rate and low temperature is desired. A high growth rate is typically achieved by increasing the NPS flow at fixed pressure and constant hydrogen carrier flow. This requires a commensurate increase in methylsilane flow to keep a high carbon concentration. Because increasing the methylsilane flow was limited by the methylsilane flow controller, we decreased our hydrogen flow while holding the NPS and methylsilane flows constant to accomplish the same effect. When we decrease the hydrogen flow, at fixed methylsilane/NPS flow ratio, we are increasing both the partial pressure of NPS and methylsilane, hence growth rate, leading to an increased carbon fraction. Once we were no longer able to decrease the hydrogen flow, we instead reduced the NPS flow to increase carbon levels. In figure 4, we compare the carbon levels measured by SIMS and XRD versus the methylsilane/NPS flow ratio for two different hydrogen carrier flows. We are increasing the carbon levels by increasing the ratio of methylsilane to NPS flow, even though we are decreasing the NPS flow.

The substitutional carbon percentage calculated from XRD was then compared with the total carbon percentage determined from SIMS. Note that non-substitutional carbon is observed to create deep levels in silicon [11]. This will

**Table 1.** Comparison of fully substitutional carbon % in silicon among different precursors.

| Precursor | Silane [2] | Silane [8] | Disilane [13] | NPS (this work) | NPS (this work) |
|---|---|---|---|---|---|
| Carbon fraction (%) | 1.8 | 1.44 | 2.35 | 1.8 | 2.1 |
| Growth rate (nm $\min^{-1}$) | N/A | 0.3 | N/A | 18 | 13 |
| Temperature (°C) | 550 | 550 | 525 | 575 | 575 |
| Tensile strain (%) | 1.05 | 0.85 | 1.35 | 1.05 | 1.23 |

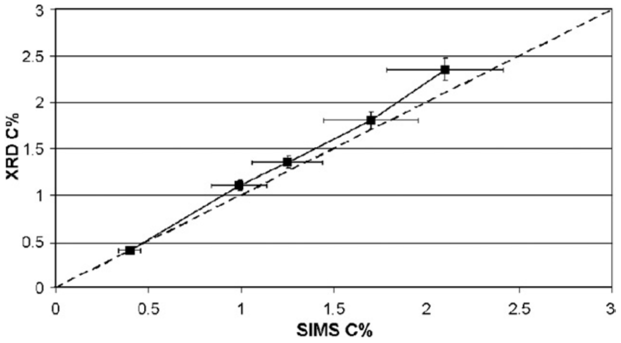

**Figure 5.** A comparison of substitutional carbon percentage measured from XRD versus total carbon percentage determined by SIMS. Relative error bars of 5% and 15% were used for the XRD and SIMS measurements, respectively.

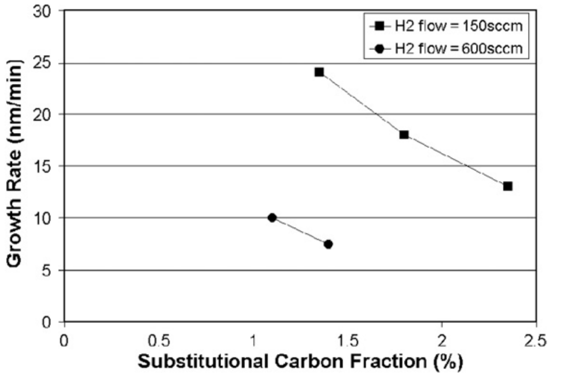

**Figure 6.** Plot of substitutional carbon % versus growth rate. Growth conditions were at 6 Torr. and 575 °C, with constant methylsilane flow of 1 sccm. The squares represent a hydrogen flow of 150 sccm, and the circles represent a hydrogen flow of 600 sccm. The decrease in growth rate is due to a decrease in the NPS source flow.

severely degrade the electronic properties of the films grown. In figure 5 we compare substitutional carbon (XRD) versus total carbon (SIMS) for growth conditions at 575 °C, in a chamber pressure of 6 Torr, with varying NPS, methylsilane and hydrogen flows. It can be inferred that fully substitutional carbon percentages up to 2.1% have been achieved.

Figure 6 shows the growth rate versus substitutional carbon fraction for different hydrogen carrier flows. It appears that the growth rate decreases at high carbon levels. This was a side effect of how we raised the carbon level as described earlier, i.e., by decreasing the NPS flow. Due to the limited maximum methylsilane flow lowering the NPS flow reduced the growth rate.

For the future, we would like to be able to increase both the methylsilane flow to allow higher carbon fraction and higher NPS flows to achieve higher growth rates at high substitutional carbon percentages.

Atomic force microscopy (AFM) surface scans of 50 $\mu$m × 50 $\mu$m squares were done on samples with substitutional carbon fractions of 1.3% and 2.1%. The growth rates of these samples are 24 nm $\min^{-1}$ and 13 nm $\min^{-1}$ respectively, with a thickness of 180 nm and 130 nm, respectively. The rms roughnesses for these samples is 2.5 nm and 5 nm respectively, compared with a 0.7 nm rms roughness from a NPS silicon epitaxy sample. The increased surface roughness may be attributed to increased disorder on the surface due to high carbon percentages.

Comparison of our work to other reports of fully substitutional carbon with high carbon percentages by CVD is shown in table 1. For carbon fractions in the range of 1.5% or higher, the highest reported rates were only 0.3 nm $\min^{-1}$, versus 18 nm $\min^{-1}$ at 1.8% and 13 nm $\min^{-1}$ at 2.1% in this work. Thus we have achieved the same substitutional carbon percentages at a slightly higher temperature and much higher growth rate (table 1), although very little on growth rates has been reported. Higher temperature growth of $Si_{1-y}C_y$ alloys may actually be desirable as it has been shown that it is easier to accomplish selective silicon growth at higher temperatures [12].

## Conclusions

High quality $Si_{1-y}C_y$ alloy layers were achieved using neopentasilane as the silicon source with methylsilane. Growth rates of $Si_{1-y}C_y$ alloys of 18 nm $\min^{-1}$ and 13 nm $\min^{-1}$ for fully substitutional carbon levels of 1.8% and 2.1%, respectively, were achieved. These are the highest growth rate reported for high fully substitutional carbon percentages in a LPCVD system. The highest substitutional carbon level achieved was 2.6% (strained perpendicular lattice constant of 5.347 Å) as determined by x-ray diffraction.

## Acknowledgment

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