Boron and Carbon co-doping in high percentage Silicon-Germanium Alloys - Effects of Dopant Incorporation, Strain Compensation and Microstructure -

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1. Introduction

State-of-the-art CMOS technology relies on the use of embedded and/or liner stressors to boost performance. Generally, the channel carrier mobility can be enhanced by uniaxial strain applied to the channel volume by pseudomorphically growing highly-strained selective epitaxial layers into the adjacent source drain (S/D) regions. This method has been successfully employed in 90, 65, 45 and recently in 32 nm CMOS products including microprocessors. However, scaling of device dimensions in successive nodes has reduced the effective gate pitch and therefore, has led to an ever decreasing available volume for embedded stressor material in the source/drain areas. This results in strain loss in the channel. Consequently, the channel strain of a previous generation can only be maintained in a following node if the embedded stressors are made of materials with an appropriately higher stress. Furthermore, a performance gain over the previous generation requires even more strain to compensate for the volume loss due to scaling. Fortunately, high strain is readily achieved in embedded silicon-germanium by simply increasing the germanium concentration.

In this paper we discuss the epitaxial growth, dopant incorporation, strain compensation due to the dopants and defect generation in high strain SiGe layers. We study the interfering effects of boron and carbon co-doping and investigate how the dopants are incorporated into the lattice during epitaxial growth.

2. Experimental

In-situ boron doped, carbon doped and boron-carbon co-doped $Si_{40\%}Ge_{60\%}$ films were epitaxially grown on n-type silicon wafers in a commercial 300 mm RPCVD reactor with different amounts of boron and/or carbon doping. The films were deposited at low temperature to achieve high doping levels and avoid thermally induced relaxation. A thickness range of 20 to 27 nm was chosen to retain a fully strained layer while allowing sufficient material for physical and electrical analyses. The films were characterized by scanning (SEM) and transmission electron microscopy (TEM), x-ray diffraction (XRD), atomic force microcopy (AFM), Secondary Ion Mass Spectrometry (SIMS), and four-point probe measurements.

3. Results and discussion

An undoped 20nm thick epitaxially grown non-relaxed layer of $Si_{40\%}Ge_{60\%}$ exhibited a strain of 2.34% as measured by XRD. Adding boron and/or carbon to the $Si_{40\%}Ge_{60\%}$ lowered the measured strain due to the smaller size of the boron and carbon atoms (Figure 1).



Figure 1: Decreasing strain in carbon doped $Si_{40\%}Ge_{60\%}$; all carbon is incorporated substitutionally up to at about $6x10^{20}$ cm⁻³ (1.2 atomic%), above which part of the additional carbon is also incorporated at interstitial sites

Samples with boron concentrations ranging from $8 \cdot 10^{19} \text{ cm}^{-3}$ to $2 \cdot 10^{21} \text{ cm}^{-3}$ and carbon concentrations from $3 \cdot 10^{19} \text{ cm}^{-3}$ to $8 \cdot 10^{20} \text{ cm}^{-3}$ were grown under the same deposition conditions as undoped films with the exception of the addition of monomethylsilane and/or diborane to the gas mixture. The partial pressure of the dopant gases was 150 to 1500 times smaller for monomethylsilane and 12.000 to 100.000 smaller for diborane than the partial pressure of the process gases, therefore maintaining similar deposition conditions for each grown layer. The partial pressure of monomethylsilane was 10 to 1000 times higher then the

partial pressure of diborane. The first observed effect in boron and carbon co-doped samples was that at the same dopant gas partial pressure ratio boron is much easier incorporated than carbon. Studies with constant boron doping in the layer by varying the monomethylsilane partial pressure showed that the carbon incorporation is reduced with increased boron. This is partly an effect of the increased growth rate due to the addition of more diborane to the gas mixture allowing less time for carbon incorporation. In addition, it is observed that at no or lower boron co-doping the graph is more non-linear indicating an initial substitutional carbon incorporation followed by non-substitutional incorporation at higher carbon concentrations. At high boron concentrations carbon seems to incorporate preferred at interstitial sites (linear incorporation behavior) since the substitutional sites are mostly incorporated by boron atoms. This postulation is supported by other measurements and will be discussed in detail in the presentation.



Figure 2: Boron incorporation into constant carbon doped $Si_{40\%}Ge_{60\%}$ as measured with Secondary Ion Mass Spectrometry (SIMS)

A study with constant carbon in the layer showed that with increased diborane partial pressure the amount of incorporated boron increases more the higher the carbon concentration in the layer. As mentioned above, the increased boron incorporation may be partly a result of the decreased growth rate due to the higher monomethylsilane partial pressure (Figure 2) Also, a linear incorporation behavior is observed at boron doping levels up to about $1 \cdot 10^{21}$ cm⁻³. Around and above $1 \cdot 10^{21}$ cm⁻³ an increased boron incorporation is observed, coinciding with the formation of point defects observed in transmission electron micrographs (Figure 3) and a raise in resistivity. Boron may be incorporated in interstitial sites or forms clusters.

Strain compensation due to boron or carbon was observed in both doping cases although the microstructure was different. Boron doping lead to the formation of perfect misfit dislocations, which relaxed the Si_{40%}Ge_{60%} layer. With increased boron an increasing dislocation density was observed. Above 1.10²¹ cm⁻³ the dislocations began to dissolve and point defects start to form (Figure 3). Carbon incorporation generated only point defects, no crystalline defects were observed by TEM. In the co-doped case the interaction and defect formation became more complex. This will be discussed in detail in the presentation.



Figure 3: Plan-view transmission electron micrographs showing microstructure of boron and/or carbon co-doped $Si_{40\%}Ge_{60\%}$; left – $1.2 \cdot 10^{21}$ cm⁻³ boron only doped and right – $1.3 \cdot 10^{21}$ cm⁻³ boron and $4.0 \cdot 10^{20}$ cm⁻³ carbon co-doped.

The model for strain compensation of boron in silicon as published by Glass et. al. [1] can be applied to SiGe as well. Our measurements of boron doped $Si_{40\%}Ge_{60\%}$ show a good fit between measured and calculated strain data.

The observed strain compensation for boron and carbon co-doped Si_{40%}Ge_{60%} is additive for low boron and carbon doping values, indication both species are incorporated substitutionally. At higher doping levels the observed strain loss is not additive anymore and therefore one of the dopants must be incorporated non-substitutionally such as at interstitial sites or clusters. Using strain measurements on constant boron doped Si_{40%}Ge_{60%} with varying carbon and constant carbon doped Si_{40%}Ge_{60%} with varying boron we will answer the questions: How are boron and carbon incorporated in high percentage Si_{40%}Ge_{60%} when both dopants are present. How do they interact? Are the dopants on interstitial sites, or on substitutional sites and does one dopant push out the other from interstitial sites? When do they start to form cluster?

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5. References

[1] Glass et a., Phys. Rev. B, Vol. 61, No.11, 7628 (2000)