AN 460

High Resolution X-ray Diffraction (HR-XRD) Measurement of Substitutional Carbon in Silicon

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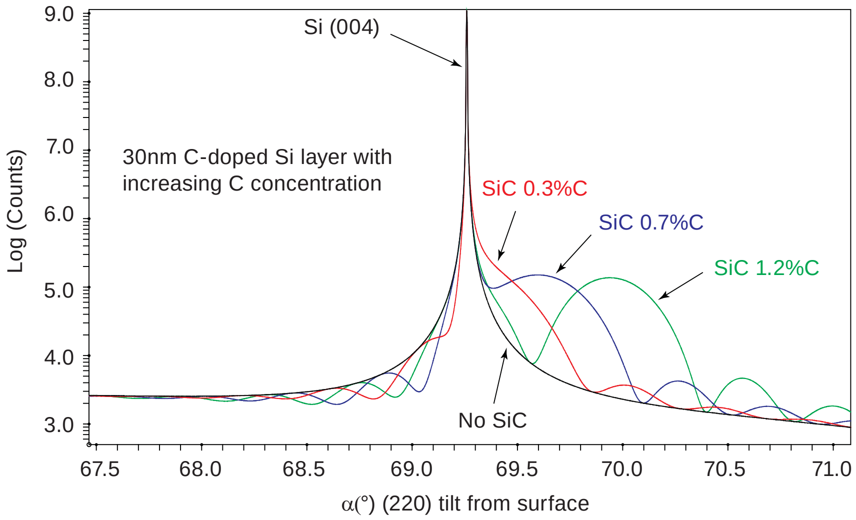
Introduction

A recent innovation in semiconductor technology is the ion implantation of carbon into silicon to create tensile strain in the silicon lattice, improving the performance of n-MOSFET semiconductor devices. In order to produce the desired effect, the carbon atoms need to be substitutional, replacing atoms in the silicon lattice. HR-XRD can be used to determine the fraction of substitutional carbon and can be combined with SIMS to characterize complex, multilayered carbon concentration profiles.

Discussion

When dopants or impurities are added substitutionally to a single crystal lattice then the lattice will be strained by the presence of the dopant atoms. In the case of a Si lattice, the presence of C atoms in the lattice results in tensile strain since the C atoms are smaller than the Si lattice atoms. This strain changes the spacing of the Si lattice, and this difference in spacing can be detected by HR-XRD.

Shown in the figure below are theoretical HR-XRD scans from Si wafers with 30nm C-doped layers containing 0.3%, 0.6%, and 1.2% C that is substitutional in the Si lattice. The peak at 69.3 degrees is from the Si lattice, while the broad peaks at higher angles represent the diffraction peaks from the Si lattice where the substitutional C is present. Because C atoms are smaller than Si atoms the lattice is under tensile strain and the diffraction peaks are shifted to the right. As the C content increases the strain also increases and the XRD peak shifts to higher angles.



XRD scans from Si with different C concentrations

One goal of ion implant and annealing studies is to determine the fraction of implanted C which becomes substitutional on the Si lattice sites under different implant and annealing conditions. SIMS analysis can measure the total C concentration in the sample (both substitutional and interstitial) while HR-XRD measures only the substitutional C. By dividing the C concentration obtained by HR-XRD by the C concentration obtained by SIMS, the percentage of the total implanted C that is substitutional can easily be calculated.

The case shown above is for a very simple system of C implanted in Si, and was modeled as a single C doped Si layer for ease of understanding. When other implanted species are added, such as P or As, then accurately describing the sample becomes more complicated due to the presence of these other elements, the damage caused by their implantation, and the requirement that these elements be electrically activated. When this is the case a multilayered XRD simulation is typically required to describe the sample. EAG can provide such simulations; however, it should be noted that XRD data alone is not sufficient to accurately describe such a sample. SIMS, TEM, and even electrical data may be required in combination with an expertly refined XRD simulation to obtain an accurate sample description.