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Deep boron diffusion induced surface damage in silicon

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ABSTRACT

This paper presents deep boron diffusion induced damages in silicon (100), (110) and (111) surfaces. The silicon (100) and (110) samples showed a broad hump at the higher angle (ω) side during x-ray Rocking curve measurement; whereas, the (111) sample shows an additional broad peak at higher angle side. All the diffused samples showed two distinct contours in reciprocal space mapping measurements. Due to the diffusion process, surface roughness of the silicon samples is found to be increased from 10 nm to 110 nm, 70 nm and 30 nm for the silicon (100), (110) and (111) samples respectively.
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1. Introduction

Doping of impurities, like B, P, As etc., in silicon is one of the most essential processes to make modern day integrated circuit devices [1–3]. Impurity doping in silicon is also being used in bulk micromachining of micro-electro-mechanical system (MEMS) fabrication process sequence [2–10]. Heavily doped boron (concentration $>5\times10^{19}$ atoms/cm^3) layer was found to have profound effect in altering the etch rate of the silicon in specific etchants [2,5,9,10]. This alteration of etch rate with doping concentration is being used as a technique to control of the thickness of micromechanical structures during bulk-micromachining or dissolved wafer processes. This technique is popularly known as etch-stop technique. It offers excellent uniformity, high reproducibility, and high yield during fabrication of MEMS structures [2,7–10].

However, doping of such high levels of boron atoms induces large stresses in the fabricated p^{++} layers based MEMS structures [10–13]. Most of the previously published reports discusses about the etch stop properties in aqueous alkaline solutions [2–10]. There are only very few reports about boron diffusion induced residual stress in silicon. The residual stresses were measured by Raman spectroscopy [10,11], wafer curvature technique [12] and bending of p^{++} Si cantilever structures [13]. But there is no reported literature on the surface damage due to the deep boron diffusion.

This paper discussed about the deep boron diffusion induced crystal damage using high resolution x-ray diffraction techniques. Surface damage due to the boron doping in silicon surfaces is studied using atomic force microscopy.

2. Experimental procedure

To study the effect of diffusion induced residual stress, three p type silicon (resistivity: 1–10 Ω-cm) wafers of (100), (110) and (111) orientations were taken. The diffusion experiment was done using Boro-Disc™ solid source at 1175 °C in a mixture of oxygen and nitrogen environment for 15 h. Detailed optimization of the deep boron diffusion to create p^{++} layer having thickness 12 μm with concentration $\geq5\times10^{19}$ atoms/cc was reported elsewhere [11]. Fig. 1 shows the secondary ion mass spectrometry (SIMS) results of the concentration profile of boron dopants in silicon (100), (110) and (111) samples, details of which were reported earlier [12]. The residual stresses were found to be in the range of 454–475 MPa, 908–963 MPa and 908–957 MPa corresponding to the silicon (100), (110) and (111) wafers respectively [11,12].

To study the crystal damage due to the boron diffusion, x-ray rocking curve measurements and reciprocal space mapping (RSM) were performed using the PANalytical PW 3050/65 X-Pert Pro MRD HRXRD system with Cu$K_{\alpha1}$ x-ray radiations source. Diffusion induced surface damage is studied by contact mode atomic force microscopy (AFM) (make: Agilent LS-5600).

3. Results and discussions

Fig. 2(a)–(c) showing the x-ray rocking curves of the silicon samples before and after the diffusion process. These

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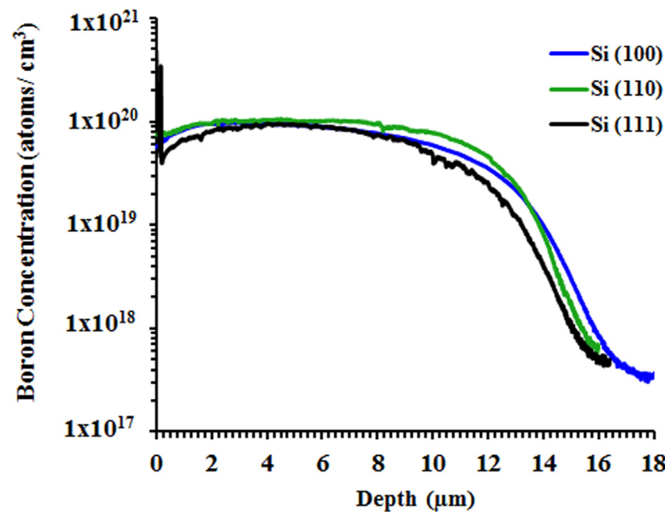

Fig. 1. Secondary ion mass spectrometry (SIMS) profiles of boron dopants (in Si wafers) diffused at 1175 °C for 15 h (reproduced by permission) [12].

measurements were done for the (400), (440), (333) planes because of their higher extinction depth for the Si (100), (110) and (111) wafers. The undoped silicon samples showed a sharp peak as expected in the x-ray rocking curve measurements of single crystal samples. After the diffusion process, the rocking curves showed broad hump appearing at the higher angle (ω) side in Si (100) and Si (110) samples, while the Si (111) sample shows an additional broad XRD peak as shown in Fig. 2(c). The broad hump in Si (100) and Si (110) samples is due to the large number of silicon interstitials, displaced during the heavy boron diffusion. Implanted samples generally show this kind of behavior [14]. In Si (111) wafer, the displaced silicon atoms may preferably segregate in interstitials sites of other set of planes as the set of {111} planes have smallest inter-planar spacing compared to the {100} and {110} planes. Thus no hump is observed in the doped (111) wafer. The additional peak in the (111) wafer at higher ω seems to be due to the formation of strained layer.

To envisage the intrinsic strain produced during the prolonged diffusion process, reciprocal space mapping (RSM) measurements are done. In RSM measurement, Q_y and Q_x axis represents the scattering vector along perpendicular and parallel direction respectively. All the diffused silicon samples showed two distinct contours in RSM measurements as shown in Fig. 2(d)–(f). The smaller contour in the RSM image arising in lower Q_y side is due to the un-doped Si regions; while large contour appearing in the higher Q_y side is boron diffused Si layer. Both the contours are not separated from each other due to its diffused interface. The RSM contour of Si (100) is showing asymmetry in the lower Q_y side (Fig. 2(d)); while the RSM contour of Si (110) is elongated along both Q_y and Q_x directions (Fig. 2(e)). This elongation in RSM of Si (110) sample seems to be due to its broadening in rocking curve measurement. This may be due to the generation of tensile strain in silicon lattice after deep boron diffusion. In Si (111) diffused sample asymmetry is very small in rocking curve and thus RSM is showing negligible elongation in lower Q_y direction of lower contour (Fig. 2(f)). Boron diffusion in Si (110) and Si (111) wafers showed prominent second RSM contours at higher Q_y side. Thus from the RSM images, one can infer that tensile strain due to the boron diffusion induces asymmetry in low Q_y direction.

Fig. 3 show the AFM images of the surfaces of the silicon wafers before and after the diffusion process. Average surface roughness of all the un-doped silicon surfaces are found to be below 10 nm as shown in Fig. 3(a)–(c). After the diffusion, average surface roughness of the Si (100), (110) and (111) surfaces are found to be 110 nm (Fig. 3(d)), 70 nm (Fig. 3(e)) and 30 nm (Fig. 3(f)) respectively. The same diffusion experiment produce different levels of surface damage in the silicon wafers of different orientations. Moreover, there are few deep craters are observed in the surfaces of the diffused samples. The numbers of these craters are also much less in Si (111) wafer compared to the other two wafers.

Previously reports suggest that silicon crystal planes show strong anisotropic behavior in surface texture in etching by alkaline solutions [5,8] and in tribological tests [15,16]. Surface damages and crater formation were also observed in implanted silicon surfaces [17,18]. Sano et al. [19] have observed the roughness of the phosphorous doped Si (100) surface. Reason for the extent of damage in different silicon crystal surfaces can be understood in the following manner.

Surface damage during the diffusion, implantation and different tribological test depends on combined effects of anisotropy of elastic constants and surface energy [17,19]. Young's modulus of Si (100), (110) and (111) wafers are reported to be 130, 169 and 180 GPa respectively [2]. The surface energy of any material depends on the density of the dangling bonds as well as how the surface atoms are attached to the bulk atoms. Crystal plane with higher density of dangling bonds can cause much instability and can lead to higher surface damage due to external loading (stress). The Si (100) surface has two dangling bonds per silicon atom hence most unstable, whereas the (110) and (111) surfaces have one dangling bond associated per silicon atom [20,21]. Though in (110) and (111) surfaces there are only one dangling bond per one silicon atom, Si (111) surface atoms are more stable due to the presence of three bonds joining with the bulk crystal. Therefore, one can expect minimum surface damage on the Si (111) surface compared to the (100) and (110) surfaces.

4. Conclusions

Deep boron diffusion is an important process step to define the thickness of the bulk micromachined silicon MEMS devices. In this study, effects of the boron diffusion in silicon (100), (110) and (111) surfaces are reported. The x-ray diffraction studies showed that in addition to the sharp rocking curve peak, the doped silicon (100) and (110) samples revealed a broad hump at the higher angle (ω) side while the (111) sample shows an additional broad XRD peak. Surface damages due to the diffusion process are also studied. Initially the surface roughness of all the silicon samples are found to be ~3–9 nm range. After the diffusion surface roughness of the (100), (110) and (111) samples are found to be 110 nm, 70 nm and

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