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Si+ Implantation into SiO_2 Layers and Ion Beam Mixing in SiO_2/Si Interfaces

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Scanning transmission electron microscopy (STEM) in combination with electron energy loss spectroscopy (EELS), soft X-ray emission spectroscopy (SXES), and cathodoluminescence (CL) have been used to investigate Si nanocluster formation in amorphous silicon dioxide layers implanted with Si+ ions. Moreover, the nanostructure of the Si doped silica films was studied by energy filtered transmission electron microscopy (EFTEM), see [1] and Fig.1 to 4. The CL measurements were performed in a Zeiss DSM 960 digital scanning electron microscope, usually with an electron beam energy E0=10 keV and a current I0≈500 nA scanned over 100x100 m. The CL light is collected via a parabolic mirror, a spectrograph (200-800 nm), and a charge coupled device (CCD) camera [2]. As samples we have used amorphous, thermally grown SiO_2 layers, 20 and 500 nm thick, wet oxidized at 1100 °C on Si substrate. The layers are of microelectronic quality and doped by Si+ ions with an energy of 12 and 150 keV and a dose of 1016 and 5×1016 ions/cm2 leading to an atomic dopant fraction of about 7 and 4 at.% at a mean depth of 20 and 200 nm, respectively, Fig.1. After high fluence Si+ ion implantation into and around the interface of the thin 20 nm a-SiO_2 layer on c-Si the formation of an ion-beam mixed buffer layer SiO_x in this region was detected by means of soft X-ray emission spectroscopy (SXES), see Fig.4, and compared with a TRIDYN computer simulation of ion implantation and ion beam mixing, [3]. This structure modulation is due to atomic knock-on and knock-off effects and respective ion beam mixing processes during the high-fluence Si+ ion implantation into the interface region, see Fig.5. Thus the buffer layer is extended over about 20 nm, even 10 nm into the Si substrate and consists mainly of an understoichiometric SiOx matrix $2 < x < 0$ with gradually decreasing of x into the Si substrate. In Si doped SiO_2:Si and understoichiometric SiO_x layers a phase separation into SiO_2 and Si clusters is observed as demonstrated already in [1]. Moreover, additional luminescence bands are observed in the green-yellow region as described in [2]. The CL spectra in the near infrared (NIR) region, Fig.6, indicate such structural changes by appearance of an additional side-band shifting towards lower energies with thermal annealing and respected Si nanocluster growth, probably, due to quantum confinement effects as we had seen previously in [2].

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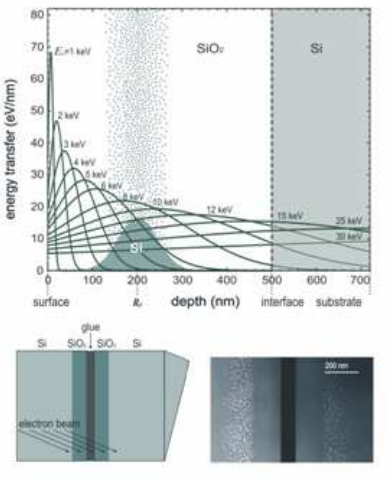

Fig. 1 Si^+ implantation profile in a 500 nm SiO_2 layer with electron excitation densities (top) and wedge sample preparation (below).

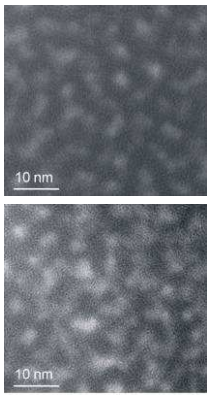

Fig. 2 EFTEM micrograph of Si clusters in a SiO_2:Si matrix after thermal annealing T_a, using the Si plasmon loss (17 eV).

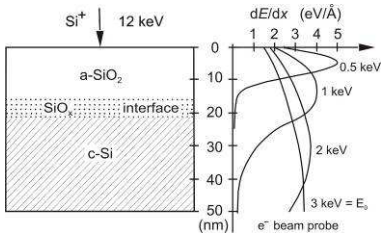

Fig. 3 Ion implantation and formation of an ion-beam mixed SiO_x buffer layer at the interface (left), and electron beam probing with a spatial excitation *dE*/*dx* (right).

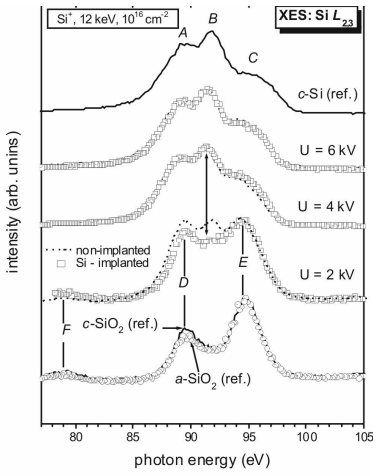

Fig.4 X-ray Si$L_{2,3}$-emission spectra of the implanted 20 nm SiO_2/Si sample in comparison to reference spectra of *c*-Si, *c*-SiO_2 and *a*-SiO_2.

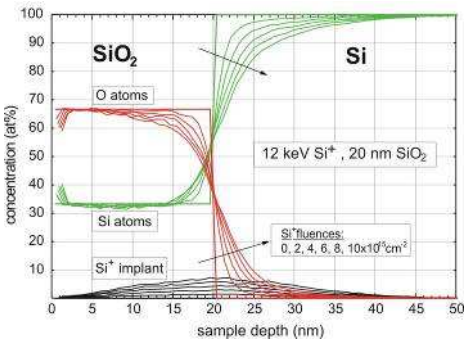

Fig. 5 TRIDYN simulation of the ion beam mixing process showing the Si^+, Si and O atom concentrations profile across the SiO_2/Si sample, [3].

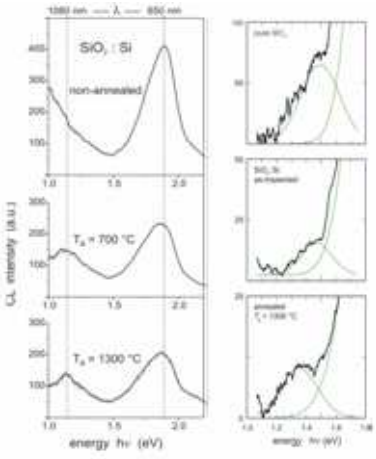

Fig. 6 Near infra-red (NIR) CL spectra of SiO_2:Si layers; the zoomed shoulder of the red band R (right) shows the shift of a sideband, probably, due to Si nanoclusters and quantum confinement effects.

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