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## Aluminum mobility and interfacial segregation in fully silicided gate contacts

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The mobility of aluminum implanted as a dopant of fully silicided nickel for advanced metal gates has been investigated following rapid thermal annealing at temperatures ranging from 160 to 700 °C. Resonant nuclear reaction profiling using the  $^{27}\text{Al}(p, \gamma)^{28}\text{Si}$  reaction was used for aluminum quantification and depth profiling. The results indicate that there is no significant aluminum loss in the whole annealing temperature interval. Furthermore, aluminum is seen to segregate near the interface with silicon oxide during metal silicidation, forming a stable layer of aluminum oxide. © 2005 American Institute of Physics. [DOI: 10.1063/1.2103392]

Intensive efforts are being directed to the development of alternative materials to continue complementary metal-oxide-semiconductor (CMOS) devices downscaling. Advances are expected from the use of alternative gate dielectric and contact materials, namely high- $\kappa$  dielectrics and metal gates. The use of fully silicided (FUSI) gated CMOS stands as a convenient choice since the starting structure is a standard polysilicon gated device, which is then reacted with an overlying metal layer, creating the metal gate. On the other hand, each particular choice of silicide presents a single work function, making it difficult to adjust the threshold voltage for both *n*-type field-effect transistors (*n*FETs) and *p*-type field-effect transistors (*p*FETs). This last difficulty can be overcome,<sup>1-3</sup> since within certain limits the threshold voltage can be finely adjusted by adding dopants to the polysilicon layer prior to silicidation.

Recently, Sb and Al dopants bonding and Sb mobility and segregation near the NiSi/SiO<sub>2</sub> interface after metal silicidation was reported, as studied by x-ray photoelectron spectroscopy (XPS) and medium energy ion scattering (MEIS).<sup>4</sup> In order to take advantage of high resolution depth profiling and other surface science techniques, inverted device structures were probed, such that the interface between silicon oxide and NiSi can then be found close to the surface (see diagram later). Medium energy ion scattering results revealed that after Ni silicidation, Sb segregates near the interface with SiO<sub>2</sub>. In addition, it was observed by XPS that Sb and Al appear in metallic and fully oxidized states, respectively. However, Al profiling near Si-containing layers is a challenging task for any ion scattering technique due to the small mass difference between Al and Si atoms. Thus, details on the aluminum depth distribution cannot be determined by MEIS and therefore the mobility of this dopant and its eventual interface segregation during metal silicidation still need clarification. This letter reports on the quantification and profiling of implanted Al atoms after thermally induced metal

silicidation using a sensitive, isotope selective, and high depth resolution profiling technique, namely resonant nuclear reaction profiling.<sup>5,6</sup>

In order to quantify implanted Al as well as to investigate its mobility and eventual interfacial segregation after Ni silicidation, two very narrow and isolated resonances in the cross-section curve of the  $^{27}\text{Al}(p, \gamma)^{28}\text{Si}$  nuclear reaction were used, namely the ones at 404.9 keV (Refs. 7 and 8) and 992 keV.<sup>9,10</sup> The former is used here for high depth resolution profiling, owing to the relatively large stopping power of protons at this intermediate energy as well as to the extremely low width of the nuclear resonance ( $\Gamma < 50$  eV). The latter presents a much larger cross section, being thus ideal for Al quantification, although leading to much lower depth resolution due to the lower stopping power of protons in this higher energy range.

Samples of the present work were prepared in an inverted Si/Ni configuration, as shown later. The thicknesses of the Ni and Si layers were conveniently chosen in order to ensure total Ni silicidation. The top silicon layer was then implanted with  $5 \times 10^{15}$  Al atoms/cm<sup>2</sup> to a projected range of 20 nm. The structures were loaded into the rapid thermal annealing unit after cleaning and HF etching, then annealed at temperatures ranging from 160 to 700 °C for 60 s at a pressure of  $6 \times 10^{-7}$  mbar, forming the NiSi structure with an overlying SiO<sub>2</sub> cap. Air exposure and residual oxygen during annealing were responsible for surface Si oxidation, forming a SiO<sub>2</sub> layer of thickness around 1 nm.

Figure 1 shows the excitation curves from the as implanted and annealed samples using the  $^{27}\text{Al}(p, \gamma)^{28}\text{Si}$  nuclear reaction near the resonance at 992 keV. Figure 2 shows the corresponding Al profiles and a sketch of the inverted Si/Ni sample configuration in the inset. These profiles were determined with a typical depth resolution of 10 nm using numerical simulations based on stochastic modeling of ion-energy loss.<sup>5,11</sup> The Al profile corresponding to the nonannealed sample perfectly matches the one obtained from a stopping and range of ions in matter<sup>12</sup> simulation of Al im-

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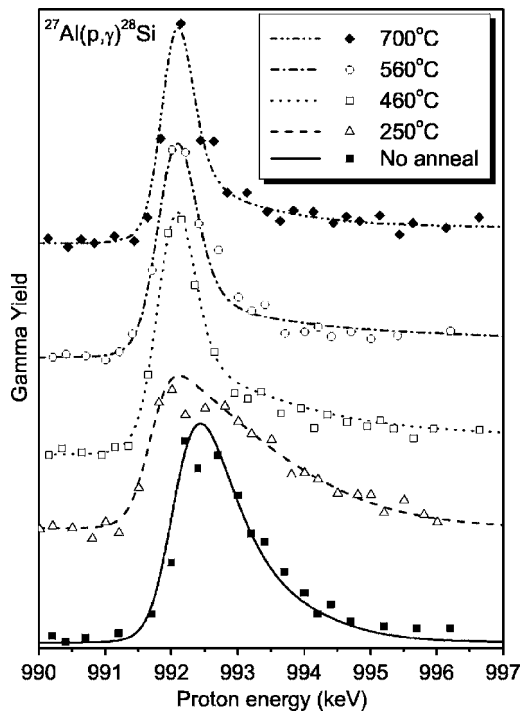


FIG. 1. Experimental (symbols) and numerically simulated (lines) excitation curves of the  $^{27}\text{Al}(p, \gamma)^{28}\text{Si}$  nuclear reaction near the resonance at 992 keV, corresponding to samples implanted with  $5 \times 10^{15} \text{Al}/\text{cm}^2$  before and after vacuum annealing at different temperatures.

planted into a Si matrix. Furthermore, one can observe that implanted Al diffuses and segregates near the sample surface during metal silicidation annealing.

The relatively poor depth resolution ( $\sim 10 \text{ nm}$ ) achievable using the nuclear resonance at 992 keV prevents one from observing interesting details about Al depth distribution near  $\text{SiO}_2/\text{NiSi}$  interface. Much better depth resolution ( $\sim 1 \text{ nm}$ ) can be achieved when using the resonance at 404.9 keV in the cross-section curve of the same nuclear reaction. Figure 3 shows the excitation curve around this resonance obtained from the sample annealed at 460 °C for 60 s. The corresponding Al profile is shown in the inset. It is noteworthy that due to the large stopping power of protons at intermediate energies, the observed peak near the resonance corresponds solely to Al located very close to the

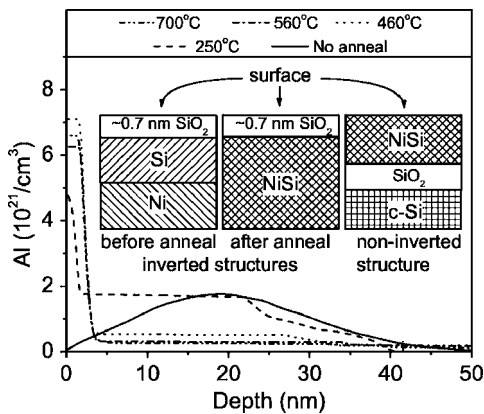


FIG. 2. Al depth profiles as determined by numerical simulation of the curves shown in Fig. 1. Sketches of the inverted device structures before and after metal silicidation as well as a noninverted FUSI structure are shown in the inset. The line styles are the same as in Fig. 1.

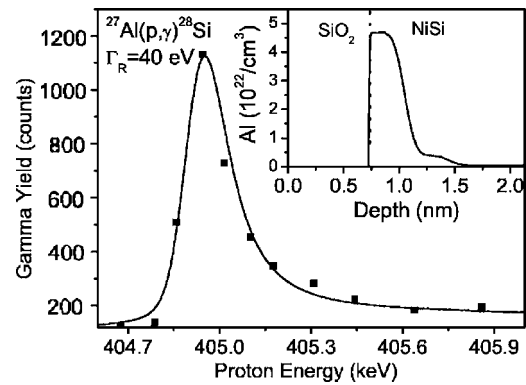


FIG. 3. High resolution ( $\sim 1 \text{ nm}$ ) excitation curve of the  $^{27}\text{Al}(p, \gamma)^{28}\text{Si}$  nuclear reaction near the resonance at 404.9 keV from the sample annealed at 460 °C for 60 s. The solid circles represent the experimental points and the solid line represents the simulated excitation curve, assuming the Al profile shown in the inset.

$\text{SiO}_2/\text{NiSi}$  interface. This is in contrast with the curves shown in Fig. 1, which reveal a constant concentration tail into the silicide layer, faraway from the maximum depth inspected in Fig. 3 (notice the different horizontal scales in the Al profiles in Figs. 1 and 3). The Al profile shows no evidence of Al penetration into the surface silicon oxide layer. Moreover, it reveals that Al atoms are segregated in a very narrow layer ( $\sim 0.5 \text{ nm}$ ) under the  $\text{SiO}_2$  cap, reproducing the behavior of Sb as a NiSi dopant.<sup>4</sup>

Figure 4 shows the total (squares) and near-surface segregated (circles) Al coverages in the NiSi samples versus annealing temperature, as determined from the excitation curves and corresponding Al depth profiles, calibrated against a 2-nm-thick  $\text{Al}_2\text{O}_3$  film on Si. Within experimental errors, no loss of Al is observed for temperatures up to 700 °C. Moreover, it is clear from Figs. 1 and 4 that aluminum segregation starts to occur at temperatures as low as 160 °C, presenting a saturation point near 380 °C. This is in contrast to what was reported for Sb as a dopant in NiSi, in which case a metallic Sb segregation peak near 400 °C, followed by substantial Sb loss at higher annealing temperatures were observed.<sup>4</sup> This contrasting behavior of Al as compared to Sb is another indication that the Al atoms that reach the NiSi/ $\text{SiO}_2$  interface oxidize, scavenging O from either the  $\text{SiO}_2$  layer, residual gas, or even from bulk poly-

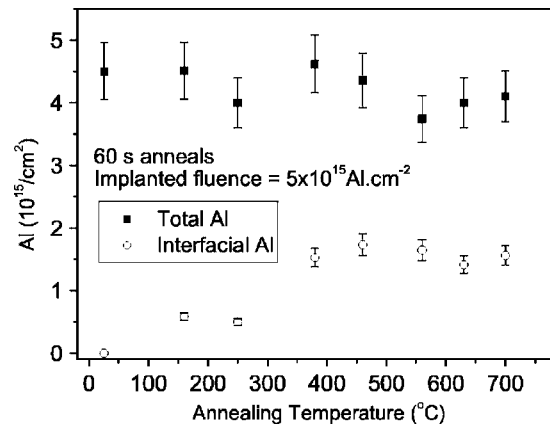


FIG. 4. (Squares): total Al areal densities as obtained from the areas under the excitation curves of the  $^{27}\text{Al}(p, \gamma)^{28}\text{Si}$  nuclear reaction. (Circles): Al segregated near the interface with the silicon oxide as obtained from integration of the near-surface peaks shown in Fig. 2.

Si/Ni to form Al<sub>2</sub>O<sub>3</sub>. Alumina on its turn, is known to be thermodynamically stable in contact with SiO<sub>2</sub>, while Sb presents a weak metallic bond to the NiSi, easily desorbing from the interface. Moreover, the reported threshold shifts for Al in NiSi are similar in sign to those reported for Al<sub>2</sub>O<sub>3</sub> films on Si.<sup>13</sup> Thus, the threshold voltage shifts are apparently caused by the thin Al<sub>2</sub>O<sub>3</sub> interfacial layer, owing to fixed charge in this layer. Other possible causes of threshold voltage shifts are diffusion during dopant activation anneals or the extended implanted Al range caused by straggling. However, this subject is still deserving further clarification.

In summary, resonant nuclear reaction profiling has been used in the investigation of Al mobility during Ni silicidation. Al atoms are seen to segregate near the SiO<sub>2</sub>/NiSi interface forming aluminum oxide within a narrow layer (~0.5 nm) close to the interface with the SiO<sub>2</sub> cap. Moreover, the Al<sub>2</sub>O<sub>3</sub> layer is thermally stable, remaining intact even for Ni silicidation carried at temperatures as high as 700 °C.

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