Polarity Effect of Electromigration in Ni_2Si Contacts on Si

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The electromigration of contacts in shallow junction devices is a reliability issue for the future very large scale integration technology. The stability of silicide contacts against a high current density is unknown. We have observed a strong polarity effect of the electromigration-induced failure at both $Ni/Ni_2Si/n^+$-Si and $Ni/Ni_2Si/p^+$-Si contact pairs. They were found to fail preferentially at the cathode. The unreacted Ni/n^+-Si and Ni/p^+-Si contact pairs have also been studied. The latter fails at the cathode while the former fails at the anode. Failure mechanisms are proposed to explain the polarity effects.

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One of the major challenges in advancing the very large scale integration (VLSI) technology is to connect a large number of transistors in a piece of Si. A dense multilevel metal wiring structure is used. In the wiring structure, most of the fine metal lines are short (a few hundred microns long). They are not connected directly to electrode pads, rather they terminate at vias and contacts. The vias are interlevel connectors. The contacts interface the metal and Si. Clearly, there are many compositional discontinuities in the multilevel structure due to interfacing dissimilar materials. These interfaces are planes of flux divergence, where electromigration damages tend to occur [1–3]. Electromigration becomes serious when current density is high. For instance, passing 1 mA through a contact area of 1 μm $\times$ 1 μm, the current density is 10^5 A/cm^2. Electromigration at these interfaces is a device reliability issue. It becomes serious for submicron VLSI structures.

When we consider contact electromigration, there are two unique feature worth mentioning besides the Si substrate whether it is n type or p type. One is current crowding due to asymmetry of the conduction path in and out of the contact, and the other is polarity. The latter is because of bias; the charge carriers can go from the metal to the Si and vice versa. Since the self-diffusivity in a metal is in general much faster than that in Si, the polarity effect may cause a large divergence in atomic fluxes from the point of view of electromigration.

While most electromigration studies focus on failures along a wire [4] or at a via [1–3,5–7], very few were about contacts [8–12], let alone the polarity effect. Since contacts are usually made of silicides, the concerns are what is the stability of a silicide contact against a high current density and how does the stability depend on the polarity effect. To answer these questions, we start with the Ni_2Si silicide. It can be formed at a low temperature, 200 to 300 °C, by interdiffusion between Ni and Si, where Ni is known to be the dominant diffusing species from marker experiments [13]. Because we know the direction of Ni diffusion in the silicide, we can use a high electrical current to enhance it or retard it. Therefore, we can study the interaction between the chemical and electrical driving forces.

In this paper, we report the behavior of Ni_2Si and Ni contact pairs on both n^+-Si and p^+-Si stressed by a current density up to 5×10^4 A/cm^2. We have observed a clear polarity effect, which is extremely interesting.

The (100) Si wafers, 3–5 Ω cm, both n type and p type, were oxidized to a thickness of 300 nm oxide. The optical photolithography and buffered HF etching were used to define and etch the Si channel region in the oxide. A screen oxide was grown to 20 nm thick for ion implantation. The wafers were ion implanted with dosage 5×10^{15} ions/cm^2 of As^+ and ${BF_2}^+$ accelerated to 40 keV into (100) p-Si and n-Si substrate, respectively. Anneal at 900 °C for 30 min in N_2 ambient was followed to activate and drive in As^+ and ${BF_2}^+$ dopants. The sheet resistances of the n^+-Si and p^+-Si were 35.7 and 26.7 $\Omega/\square$, respectively. A 300 nm low temperature oxide was then grown on the n^+/p junctions and the p^+/n junctions. The 10 μm $\times$ 10 μm contact windows were opened to the junction region by photolithography and buffered HF etching. Finally, Ni films were deposited to a thickness of 260 nm. The Ni bond pads were defined by photolithography with a lift-off process in acetone. The specific contact resistivities of the Ni/n^+-Si and Ni/p^+-Si contacts are 7.2×10^{-6} and 6.7×10^{-6} Ω cm^2, respectively. Shown in Fig. 1 are the top view and side view of the test structure. The negative contact (cathode) is defined as the contact where electrons flow from the metal into the Si. The positive contact (anode) is the one where electrons flow from the Si into the metal.

We prepared the Ni/n^+-Si and Ni/p^+-Si samples with and without thermal anneal for the contact reaction study. The samples annealed at 275 °C in a vacuum tube of 10^{-7} torr will form Ni_2Si at the contacts [13]. We used different anneal times (3.25, 6.75, 15, 30, and 48 h) to grow different thicknesses of the Ni_2Si. After the 30 h annealing, formation of Ni_2Si in the

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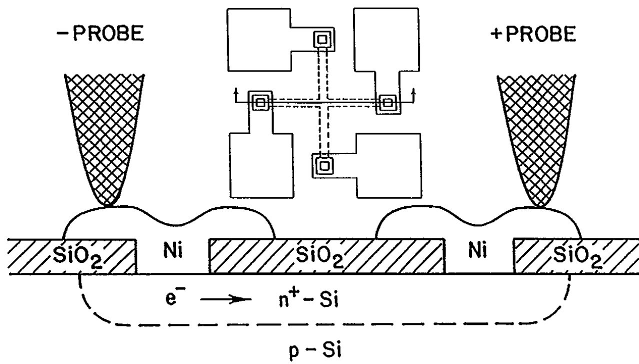

FIG. 1. The side view of the test structure used for contact failure studies (the inset in the middle shows the top view). An Ni/n^+-Si contact is shown.

contact areas is complete. The stability of the nickel silicide contacts under electrical stress was monitored by contact resistance changes. Morphological changes were examined by scanning electron microscopy (SEM).

The stress temperature for the annealed and unannealed contacts was 275 °C. The optical inspection was made *in situ*. The samples were stressed until damage occurred. The damage is defined as contact degradation due to excessive silicide formation. The degraded contacts appear black in the optical microscope. The failure time is defined as the time for the whole contact to be damaged.

(1) $Ni/Ni_2Si/n^+$-Si and $Ni/Ni_2Si/p^+$-Si contacts.—The completely reacted $Ni/Ni_2Si/n^+$-Si and $Ni/Ni_2Si/p^+$-Si contact pairs were stressed at current densities ranging from 3×10^4 to 5×10^4 A/cm^2. A total of 177 contact pairs of $Ni/Ni_2Si/n^+$-Si has been tested. It was found that 70% of the damage occurred at the negative contacts, 18% at the positive contacts, and 12% at both contacts. Figures 2(a) and 2(b) are the SEM images of the tested samples exhibiting damage at the negative contacts. Figure 2(a) shows clearly the polarity effect of damage. The surface morphology of the damaged negative contact is shown in Fig. 2(b). For the stressed $Ni/Ni_2Si/p^+$-Si contact pairs, similar failure behavior was found from a total of 100 samples. About 68% exhibited damage at negative contacts, 11% at the positive contacts, and 21% at both contacts.

(2) Ni/n^+-Si and Ni/p^+-Si contacts.—The unannealed Ni/n^+-Si and Ni/p^+-Si contact pairs also show a polarity effect in contact degradation. Interestingly, for the Ni/n^+-Si, the positive contacts reacted while the negative contacts remained intact. On the contrary, for the Ni/p^+-Si, silicide reaction occurred at the negative contacts but there was no reaction at the positive contacts. Figures 3(a) and 3(b) show the surface morphologies of

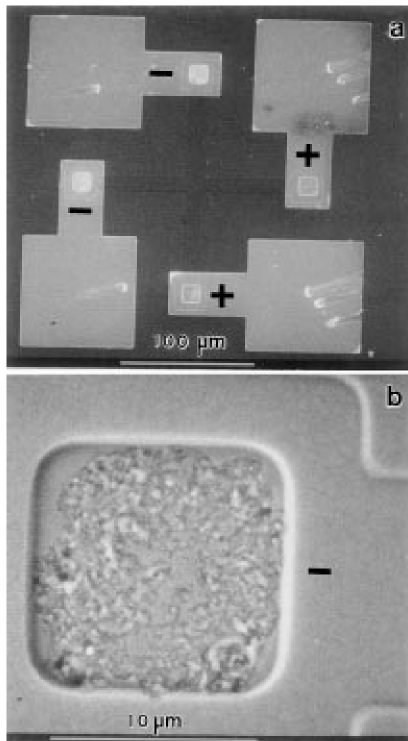

FIG. 2. Scanning electron micrographs depicting failures at $Ni/Ni_2Si/n^+$-Si contacts after electrical stressing (5×10^4 A/cm^2) at 275 °C. The polarity effect can be clearly seen in (a). The damage preferentially occurred at the negative contacts. (b) shows the surface morphology of silicide formation at the negative contact.

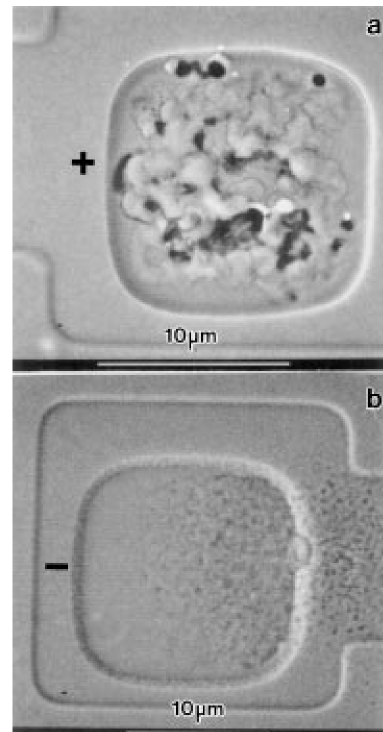

FIG. 3. SEM micrographs showing (a) the damaged positive Ni/n^+-Si contact and (b) the damaged negative Ni/p^+-Si contact stressed at 275 °C.

the damaged positive Ni/n^+-Si contact and the damaged negative Ni/p^+-Si contact, respectively. In comparison with the previous Ni/Ni_2Si/n^+-Si and Ni/Ni_2Si/p^+-Si cases, the unannealed contact pairs showed a stronger polarity effect in terms of a higher percentage of failure, as shown in Tables I and II.

(3) Partially reacted Ni/Ni_2Si/n^+-Si and Ni/Ni_2Si/p^+-Si contacts.—Figure 4(a) illustrates the failure times of the completely reacted (48 h anneal at 275 °C), the partially reacted (3.25 and 6.75 h anneals at 275 °C), and the unreacted n^+-Si contact pairs as a function of the applied current density. Figure 4(b) shows the failure times of the completely reacted (48 h at 275 °C), the partially reacted (17.5 and 24 h at 275 °C), and the unreacted p^+-Si contact pairs. It shows a correlation between the failure time and the thickness of the Ni_2Si. The completely reacted Ni/Ni_2Si/n^+-Si and Ni/Ni_2Si/p^+-Si contact pairs exhibit an earlier failure than the partially reacted under the same current density. Tables I and II summarize the statistics data for the completely, partially reacted, and unreacted contact pairs of the n^+-Si and p^+-Si, respectively.

To explain the above results, we note that on the basis of the large difference between atomic diffusivity in Si and in Ni or in Ni_2Si, we should expect failure to occur on the positive contacts. It is the same as the wear-out mechanism of Al at a W contact [1–3,5,6]. The electrons will drive Ni away from the positive contacts and lead to opening; it does happen in the Ni/n^+-Si samples. However, other samples fail predominantly at the negative side, indicating different failure mechanisms. We note that all the polarity effects observed here are net results of competing events occurring between the positive and negative contacts. One of them tends to dominate.

Consider the Ni_2Si/n^+-Si contact pairs. As a current is applied, at the negative contact the electrons flow in the same direction as the Ni diffusion. Some of the Ni atoms will electromigrate from Ni_2Si into Si interstitially. These Ni atoms are removed from the silicide but they can be replenished from the Ni bond pad, so no net energy is spent to decompose and reform the compound. Solute atoms of Ni in Si are known to dissolve and diffuse interstitially. These Ni interstitials weaken the covalent bonds of those interfacial Si atoms and allow them to break away from the Si lattice [14]. The mobile Si atoms can react with Ni_2Si to form NiSi and $NiSi_2$. The NiSi or $NiSi_2$ silicide has a high resistivity [15] and large temperature coefficient of resistivity. Eventually the contact fails due to a high rate of excessive silicide formation. At the positive contact, the electrons flow against the Ni diffusion in Ni_2Si. To drive Ni atoms from Ni_2Si into the Ni bond pad, an energy is needed to decompose the silicide. Also, it is against the Ni concentration gradient to drive Ni from the Ni_2Si to the Ni pad. Hence, the reaction in a positive contact is much less than that in a negative side, so we expect the failure to occur predominantly in the negative contacts. We have the observed polarity effect of Ni_2Si/n^+-Si.

In the case of Ni_2Si/p^+-Si contact pairs, we expect they behave similarly to the Ni_2Si/n^+-Si discussed above. However, we note that there is an important difference between the positive and negative ones. Electrons and holes must be combined at the negative contacts, but they must be generated at the positive contacts. We speculate that when a large number of them are combined at an interface, the energy release will create Joule heating to enhance the interfacial reaction. We also note that in a direct band-gap semiconductor such a recombination may lead to light emission. But for Si, which has an indirect band gap, the energy release will be absorbed by phonons. On the other hand, the generation of electron-hole pairs at a positive contact would spend energy and retard the interfacial reaction. Hence, the negative contacts fail predominantly. This is also true for the unreacted Ni/p^+-Si.

For the unreacted Ni/n^+-Si, the failure occurs at the positive contacts, as expected from the wear-out mechanism. Nevertheless, we should note that the decomposition mechanism (for the Ni_2Si/n^+-Si contacts) cannot explain the failure observed here because no silicide has been thermally formed prior to current stressing. At the negative contacts, the electromigration-assisted Ni diffusion from Ni into Si is slow compared to the case of Ni_2Si/n^+-Si. The silicide formation is sluggish and

TABLE I. Statistics of failure sites for the completely reacted (48 h annealed at 275 °C) and the partially reacted (15 and 6.75 h anneals at 275 °C) Ni/Ni_2Si/n^+-Si, and unannealed Ni/n^+-Si contact pairs.

	Total No. of stressed contact pairs	Percentage of failure sites		
		"−"	"+"	Both
275 °C−48 h	121	50%	25%	25%
275 °C−15 h	177	70%	12%	18%
275 °C−6.75 h	102	72%	9%	19%
Unannealed	120	0%	97%	3%

TABLE II. Statistics of failure sites for the completely reacted (48 h anneal at 275 °C) and the partially reacted (30, 24, and 17.5 h anneals at 275 °C) Ni/Ni_2Si/p^+-Si, and unannealed Ni/p^+-Si contact pairs.

	Total No. of stressed contact pairs	Percentage of failure sites		
		"−"	"+"	Both
275 °C−48 h	32	84%	6%	10%
275 °C−30 h	103	68%	21%	11%
275 °C−24 h	102	98%	2%	0%
275 °C−17.5 h	55	91%	9%	0%
Unannealed	120	100%	0%	0%

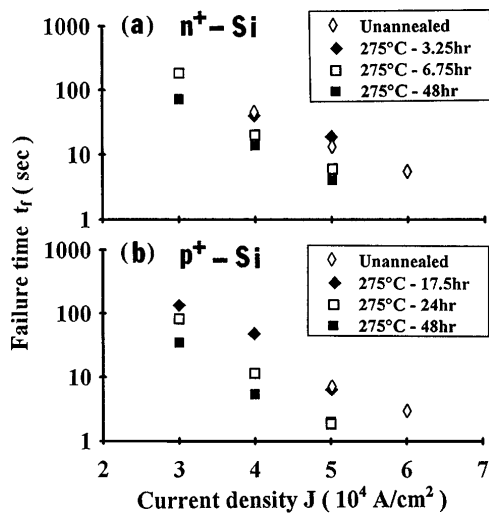

FIG. 4. Failure time of the contact pairs vs current density. (a) The completely reacted (48 h anneal at 275 °C), the partially reacted (3.25 and 6.75 h anneals at 275 °C), and the unreacted n^+-Si contact pairs. (b) The completely reacted (48 h at 275 °C), the partially reacted (17.5 and 24 h at 275 °C), and the unreacted p^+-Si contact pairs stressed at the current densities ranging from 3×10^4 to 5×10^4 A/cm^2 at 275 °C.

the tendency of failure is reduced. This is because the activation energies of diffusion of Ni in Ni_2Si and Ni are 1.24 [16] and 2.9 eV [17], respectively.

For the partially reacted $Ni/Ni_2Si/n^+$-Si and $Ni/Ni_2Si/p^+$-Si, their behaviors are in agreement with the explanation given in the above. They tend to fail faster than the unreacted contacts, but slower than the fully reacted. The behavior change can be explained by two reasons. First, Ni atoms can diffuse faster in Ni_2Si than in pure Ni. Second, nickel silicide has a higher resistivity and larger temperature coefficient of resistivity than pure Ni.

Besides the polarity effect, we have detected current crowding phenomena. Current crowding is especially evident in the unreacted Ni/p^+-Si contact pairs. We observed this event during the contact degradation. The silicide reaction originates from the leading edge of the negative contact, the edge which is closer to the positive side. Then it spreads out slowly over the entire contact area. Moreover, in the unreacted interface, the residue native Si oxide may also cause local current crowding. The Joule heating associated with the thermal runaway and the current runaway will sometimes melt the contact.

Statistically not all the contacts are made the same due to variation in processing control; we expect minor deviation in the contact behavior especially when it is affected by the native Si oxide. The native oxide not only causes current crowding but also changes the rate and uniformity of silicide formation.

We cannot use Joule heating alone to explain the polarity effect observed in contacts on n^+-Si. This is because the probabilities of failure on both positive and negative contacts due to Joule heating should be the same. On p^+-Si, the energy change due to electron-hole recombination must be included in our consideration. So far, we have not discussed the structural information about the silicide formation. Our preliminary results of transmission electron microscopy support the explanations given in the above.

In conclusion, we have studied the stability of Ni_2Si and Ni contacts on both n^+-Si and p^+-Si stressed by a high current density up to 5×10^4 A/cm^2. A clear polarity effect has been found. On Ni_2Si/n^+-Si, the contact failure is controlled by electromigration-assisted Ni diffusion into Si that occurs preferentially at the negative contacts. But on Ni/n^+-Si contacts, it is controlled by electromigration-assisted Ni diffusion away from the Si at the positive contacts. On p^+-Si, the electromigration-assisted reaction and the electron-hole recombination effect contribute to the dominate failure in the negative contacts.

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