TiSi$_2$ phase transformation characteristics on narrow devices

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Abstract

Accurate prediction of TiSi$_2$ transformation requires test structures with small silicided surface areas. To evaluate the area dependence of the C49 to C54 transformation, a new monitor was developed with minimal silicide surface area. Small area structures were found to exhibit a bimodal resistance distribution that was nearly insensitive to process transformation conditions. Starvation for C54 nucleation sites resulted in a high frequency of non-transformation even at high annealing temperatures. Transmission electron microscopy analysis showed that the Ti silicide in these structures is either C49 or C54 phase, with little or no mixed phases present. A cooperative C54 nucleation mechanism is proposed to explain this phenomena. The presence of small quantities of a molybdenum impurity such as molybdenum during silicide formation has been found to increase the availability of C54 forming nuclei by two orders of magnitude. The molybdenum acts as a catalyst and does not require interface mixing or the creation of an amorphous Si layer to enhance nucleation. The addition of molybdenum has been demonstrated to eliminate the bimodal resistance distribution.

Keywords: Titanium silicide; Nucleation

1. Introduction

Titanium silicide is widely used as a self-aligned silicide because of its properties of low resistivity and relatively good thermal stability. It is generally accepted that TiSi$_2$ initially forms in the metastable C49 phase (60–90 μΩ cm) which must be transformed through additional thermal treatment to the desired low resistivity C54 phase (12–20 μΩ cm) [1,2]. Transformation of TiSi$_2$ to the low resistivity C54 phase is nucleation limited, requiring a high activation energy >5.6 eV on single-crystal (100) silicon [3]. Factors that influence the phase transformation kinetics include TiSi$_2$ film thickness, surface energy, and formation temperature. Transformation of TiSi$_2$ from C49 to C54 phase is more difficult for small structures due to the limited availability of nucleation sites. If the transformation is incomplete or nonuniform, a degradation in circuit performance is observed. The RC delay associated with lack of phase transformation is as much as 5–10% in high performance circuits, depending on specific layout. Stage delay for a typical ring oscillator is modeled in Fig. 1 as a function of gate-conductor sheet resistance. A morphological degradation, referred to as agglomeration, may occur if the thermal treatment for transformation is excessive, causing discontinuities in the silicide.

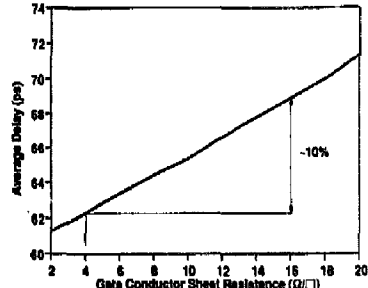* Corresponding author. Tel: 802-769-9651. Fax: 802-769-9659. E-mail: Mad__Dog@vnet.ibm.com.

Fig. 1. Ring oscillator stage delay of a CMOS inverter circuit as a function of gate conductor sheet resistance.

As reported by Lasky et al. [4], conversion of TiSi$_2$ to C54 phase is more difficult on narrow lines due to the scarcity of C54 forming nuclei. In blanket TiSi$_2$ films, a typical C54 grain size is 5–25 μm depending on formation conditions and film thickness; while, for structures much narrower than 10 μm, Lasky observed that C54 grain size is about twice the line width. From statistical arguments, it was postulated that a higher density of nuclei is required to complete the transformation on narrow structures. We have found that the total surface area of a test structure, not just the line width, affects transformation. A narrow resistor with large silicided pads attached may be completely transformed under typical processing conditions, while an identical resistor without large

pads will exhibit a bimodal sheet resistance (RS) distribution. The geometry of the RS test structure is an important parameter for accurately monitoring silicide behavior.

2. Experimental

Samples were prepared by depositing 300 nm polysilicon over 10 nm of oxide on p-type (100) silicon wafers. After line patterning, the polysilicon films were doped with either boron or phosphorus at doses in the range of 1×10^{15} to 4×10^{15} cm^{-2} and activated by rapid thermal annealing (RTA). Following Ti deposition (45 nm), silicide formation was performed by either tube furnace annealing (650 °C) or RTA (725 °C) in N_2. After TiSi$_2$ formation, unreacted Ti was selectively etched, followed by a high temperature anneal in N_2 to induce C54 transformation. Microprobing of individual silicided poly–Si lines in a typical circuit (0.5 μm line width, 30 μm^2 area) indicated that approximately half the lines were four times higher in resistivity. The resistivity delta was due to some lines not converting to C54 TiSi$_2$. The sheet resistance (RS) distribution was bimodal, with the first population forming a Gaussian distribution with a mean of 3 Ω/□. The second population was also Gaussian with a mean of 12 Ω/□.

The fraction of lines converted to C54 was relatively insensitive to TiSi$_2$ transformation anneal; the transformation annealing conditions ranged from extended furnace annealing at 750 °C for 30 min to brief RTA annealing at 920 °C. None of the conditions investigated reduced the fraction of lines in the higher resistance mode. It has been reported from studies on blanket films that higher temperatures were effective in stimulating C54 transformation [5]. In contrast, we found that higher temperature transformation annealing did not produce effective C54 conversion on typical device structures. TiSi$_2$ formation by RTA and higher temperature furnace formation anneal did, however, increase conversion in the subsequent transformation anneal, but did not entirely eliminate C49 phase TiSi$_2$. Formation at higher temperatures must be applied with caution as an undesirable degree of TiSi$_2$ bridging may result.

The standard bridge type (Kelvin) resistance monitors did not predict that there was a significant fraction of polycide lines not converted to C54 phase. The monitors consisted of minimum width poly–Si lines connected to large silicided pads (100 × 100 μm^2) designed to be probed during post silicide test. The monitor shown in Fig. 2 (Type 1), indicated that all TiSi$_2$ was completely transformed. The ability to form the C54 phase appears to be influenced by the silicided surface area of the entire monitor, not just the area between the inner arms of a bridge-type resistor.

A new resistance monitor was developed to investigate the apparently different behavior between "probing" monitors with large pads and "isolated" lines. The monitor (Fig. 2, Type 2), which is not attached to any adjacent silicided pads, is wired via contacts and cannot be tested until the first metal level. Fig. 3 compares RS data from 32 × 0.6 μm N$^+$ poly–Si probing and isolated monitors. Only the isolated monitor shows a bimodal RS distribution. The clean bimodal distribution implies the absence of partially converted TiSi$_2$; the lines are either C49 or C54 phase, with little or no mixed phase present. Transmission electron microscopy analysis
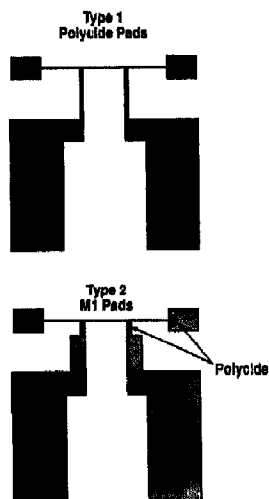

Type 1
Polycide Pads

Type 2
M1 Pads

Polycide

Fig. 2. Comparison of probing (Type 1) and isolated (Type 2) RS monitor configurations.

(a)

C54

C49

Frequency

Sheet Resistance (Ω/□)

(b)

C54

C49

Frequency

Sheet Resistance (Ω/□)
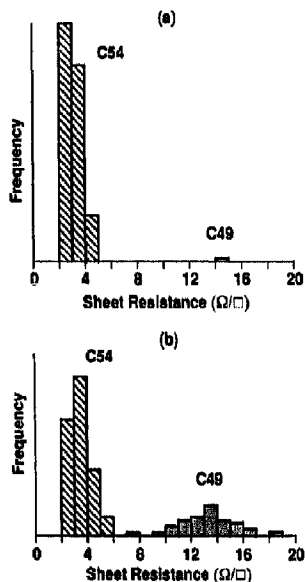
Fig. 3. Sheet resistance of (a) probing and (b) isolated RS monitors (32 × 0.6 μm) with N-polycide (tube-furnace formation at 650 °C).

was used to verify that only a single phase was present in each structure. This contrasts with previously reported data that narrow lines contain mixed C49/C54 with the fraction of C49 increasing at narrower widths [6].

3. Discussion

3.1. Cooperative nucleation

The presence of a single phase in each structure appears to represent a different phenomena than nucleation site limited C54 transformation. It is statistically improbable that some sites would have no nucleation events (C49 phase), while other sites would be saturated with nuclei (C54 phase). Since the isolated RS monitor is long enough to contain many C54 grains, the fact that partially converted structures were not found suggests a cooperative phase transformation mechanism. It is postulated that C54 grains are acting as nucleation sites for adjacent C49 grains, causing C54 to propagate across the entire structure. This mechanism explains the easy conversion of the probing (Type 1) monitor in terms of C54 grains forming in the large pad areas (where a nucleation event is statistically more likely), propagating conversion of the entire structure. We call this effect cooperative nucleation.

3.2. Calculation of C54 nucleation density

Test structures with isolated diffusions of various widths and critical areas were used to investigate C54 nucleation in greater detail. Structure areas were 22–100 μm^2 with the length held constant at 20 μm and width varied from 0.4 to 3.0 μm. Processing conditions were the same as in the preceding case, with silicide formation performed either in a tube furnace or by RTA; the transformation anneal was by RTA. It was generally found that larger area structures had a higher fraction of sites transformed to C54 phase, as would be consistent with a nucleation site limited/cooperative transformation process. The fraction transformed was a strong function of dopant type and TiSi$_2$ formation method. As seen in Fig. 4, C54 transformation on N-type diffusions was incomplete over the range of formation conditions used. In contrast, transformation on P-type diffusion was enhanced by RTA as compared to furnace formation. With RTA formation, all P-type areas > 30 μm^2 were transformed.

Data collected from these structures were used to estimate C54 nucleation density. If a Poisson distribution of C54 nuclei is assumed, the fraction of structures with at least one nucleation site may be calculated by:

$$F_T = 1 - \exp(N_d A) \tag{1}$$

where F_T is the fraction of sites in C54 phase, N_d is the nuclei density, and A the critical area. When the test structure is small relative to the propagation distance of C54 transformation, the sheet resistance distribution will be bimodal. The nucleation density can be extracted as:
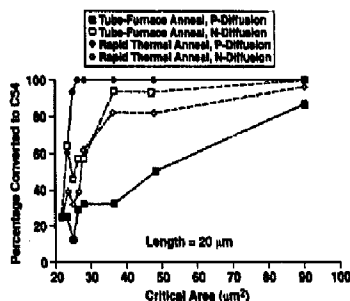

Fig. 4. C54 transformation probability on N- and P-type diffusions (tube-furnace formation at 650 °C, RTA at 725 °C).
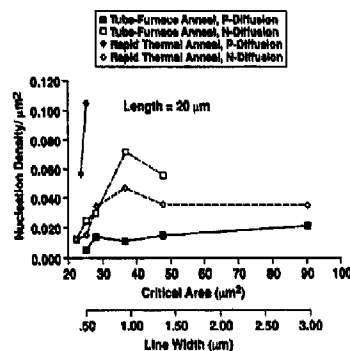

Fig. 5. C54 nucleation density on N- and P-diffusions (tube-furnace formation at 650 °C, RTA at 725 °C).

$$N_d = -\ln(1 - F_T)/A \tag{2}$$

If C54 nucleation is homogeneous, the nucleation density will be insensitive to line width. If, on the other hand, perimeter effects are influencing nucleation, the nucleation density should decrease for narrower line widths, which is typical of the so-called fineline effect. The data collected in Fig. 5 indicates that nucleation is becoming more difficult for narrower line widths where the perimeter to critical area ratio is increasing. The nucleation density appears to approach a saturation value at about 40 μm^2, corresponding to a line width of 0.9 μm. Note that surface area is not an exact multiple of line width because of the finite area required for landing contacts. The decreasing ability to create C54 nucleation at narrow line widths may be caused by TiSi$_2$ thinning at the edges or a decreasing number of available C49 grain triple points [7]. The saturation, or bulk nucleation density, is strongly influenced by formation conditions, with the greatest density apparent on P$^+$ diffusions with RTA formation. The nucleation density on P$^+$ diffusions with RTA formation could not be calculated for critical areas > 30 μm^2 because all structures had been transformed.

3.3. Effect of molybdenum impurities

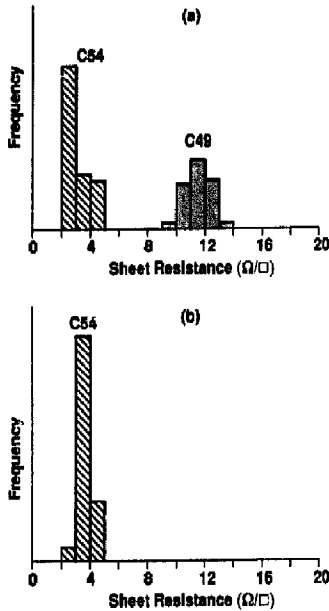A molybdenum impurity was implanted into polysilicon at energies from 15–60 keV, with doses ranging from 2×10^{13}

Fig. 6. Sheet-resistance comparison of isolated P-polycide (32×0.6 µm) RS monitor (a) without and (b) with Mo implantation.

to 1×10^{14} ions cm^{-2} prior to line patterning. The surface concentration of Mo measured by SIMS was less than 1×10^{19} cm^{-3} in all cases. Implant damage modeling (TRIM) predicted no amorphous Si layer formation with these conditions. TEM analysis of an identically implanted Si (100) wafer found few surface defects and no evidence of metallic or Mo-silicide precipitates. RS measurements taken from isolated 32×0.6 µm N- and P-type poly–Si monitors show compete conversion of the Mo implanted sample while the unimplanted control sample was bimodal. Data taken from P-type monitors is shown in Fig. 6. The average grain size of the Mo-implanted sample has been estimated by TEM to be in the order of 0.1 µm. Unimplanted monitors have grain sizes in the order of 1 µm. Assuming grain size is inversely proportional to C54 nucleation density, the metallic impurity was responsible for a two orders of magnitude increase in nucleation sites.

4. Summary

The phase transformation characteristics of TiSi$_2$ have been investigated using test structures with minimal surface area. We found that silicided surface area is a critical parameter in RS monitor design. Monitors with large surface areas will not accurately predict the RS distribution in real circuits. The ideal RS monitor should match the geometry of actual devices. Nucleation density of C54 transformation for N- and P-type diffusions has been calculated using RS monitors with small surface areas. Nucleation density was found to be dependent on the dopant and silicide formation conditions. The implantation of molybdenum prior to silicide formation has been shown to significantly enhance C54 phase transformation and improve TiSi$_2$ RS uniformity.

Acknowledgements

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