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A Quarter-Micrometer Interconnection Technology Using a TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti Multilayer Structure

Takamaro Kikkawa, *Member, IEEE*, Hidemitsu Aoki, Eiji Ikawa, and John M. Drynan

Abstract—A new interconnection structure using a TiN/Al-1%Si-0.5%Cu/TiN/Al-1%Si-0.5%Cu/TiN/Ti multilayer conductor was investigated as a quarter-micrometer interconnection candidate for 256-Mb DRAM's. It was found that intermetallic compounds such as TiAl_x were formed at both grain boundaries of Al-Si-Cu and interfaces between Al-Si-Cu and TiN of the multilayer, resulting in both increase in Vickers hardness and suppression of stress relaxation. The multilayer conductor strip, which was covered with plasma-enhanced chemical vapor deposition silicon nitride (P-SiN), suppressed stress-induced voiding after heat treatment at 500°C. Electromigration tests for quarter-micrometer wide multilayer strips indicated the improvement in the mean time to failure and the increase of the standard deviation.

I. INTRODUCTION

SINCE interconnection dimensions have been reduced, reliability failures due to stress-induced migration [1]–[6] and electromigration [7]–[9] have become more serious for aluminum (Al) conductors. It has been reported that copper addition to Al film has improved the stress-induced migration resistance [5] as well as electromigration resistance [9]. However, Al conductors, layered with barrier metals, which have been necessary for shallow junction contacts, have caused degradation in electromigration resistance because of a decrease in Al grain size [10]. Therefore, it is necessary to improve the electromigration resistance as well as the stress-induced migration resistance for Al conductors layered with barrier metals. It has been reported that Al-transition-metal compounds were effective in improving electromigration resistance [11] and that an Al/Al stacked conductor could suppress the electro- and stress migrations [12]. It has also been reported that Al films layered with titanium (Ti) or tungsten (W) films showed no hillocks after heat treatments [13] and that a Ti capping on Al conductor structure could suppress stress-induced void formation during heat treatment [14]. However, Al films layered with refractory or transition metals resulted in a resistivity in-

crease after heat treatment [15] as well as whisker formation [16]. Titanium nitride (TiN) was also used to improve electromigration resistance [16]. In addition, the TiN film was also effective for an antireflection layer on top of Al [17].

In this paper, a new layered conductor structure is investigated for quarter-micrometer interconnections. In order to fulfill requirements of high electrical and mechanical endurances, Al films are alternately deposited with a barrier of TiN. The resulting multilayer structures display good mechanical hardness and tensile strength, and long electromigration lifetimes.

II. EXPERIMENT

A barrier metal bilayer, 30-nm-thick Ti and 100-nm-thick TiN, was deposited by direct current (dc) magnetron sputtering onto oxidized (100) Si substrates, followed by consecutively sputtered 200-nm-thick Al-1%Si-0.5%Cu, 30-nm-thick TiN, 200-nm-thick Al-1%Si-0.5%Cu, 30-nm-thick TiN films without breaking the vacuum. The Ti film was deposited by Argon (Ar) sputtering at 8×10^{-3} torr and 0.4 kW without substrate heating. The 100-nm-thick TiN film was reactively sputtered with a gas mixture containing 50% Ar and 50% nitrogen (N_2) at 3×10^{-3} torr, and 2 kW at 350°C. The top and intermediate TiN films were reactively sputtered with the same gas mixture but without substrate heating. The Al-1%Si-0.5%Cu films were deposited by Ar sputtering at 6×10^{-3} torr and 7 kW at room temperature. Quarter-micrometer wide metal lines were patterned by electron-beam lithography as well as photolithography and low-temperature microwave plasma etching. The metal lines were covered with 1 μm of silicon nitride (P-SiN), which was formed by plasma-enhanced chemical vapor deposition using N_2 , NH_3 , and SiH_4 gas mixture at 0.23 torr and at 300°C as a passivation.

Ultra-micro-indentation measurements [18] were carried out. The ultra-micro-hardness was calculated from a load versus indentation depth curve for a single layer as well as for layered films. Film stresses were calculated from the wafer curvature measured by the Newton's ring method. The film composition and structure for layered metal films were characterized by X-ray diffraction analysis (XRD), transmission-electron microscopy (TEM),

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scanning-electron microscopy (SEM), and energy dispersive spectrometry (EDS). The film resistivity was measured by a four-point probe sheet resistance measurement system. Voids due to thermal and stress migrations in Al lines were observed by an optical microscope after heat treatment at 500°C. A two-dimensional finite-element modeling program was used to estimate the effect of TiN layers on Al-film stresses. Electromigration tests were conducted in a nitrogen atmosphere for Al stripes without passivation layer at current densities of 5×10^6 and 1×10^7 A/cm², and temperatures of 242°C and 290°C.

III. RESULTS AND DISCUSSION

A. Structural and Mechanical Properties

Cross-sectional diagrams of an Al-Si-Cu single layer, Al-Si-Cu on TiN/Ti barrier layers, and TiN/Al-Si-Cu/TiN/Al-Si-Cu alternated layers on TiN/Ti barrier layers are shown in Fig. 1(a)–(c), respectively. A TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer structure was designed as both electro- and stress-migration-resistant interconnection structure. The bottom TiN/Ti bilayer acts as a diffusion barrier between the Al-Si-Cu and the Si substrate. The thin Ti layer reduces the contact resistance between the TiN and Si substrate by forming a titanium silicide layer at the interface. The Al-Si-Cu layers are the main conducting paths. The Al-Si-Cu layer was divided into two layers in order to prevent void propagation through the Al-Si-Cu layer. A TiN thin film was used as an intermediate layer because the TiN layer reinforced the mechanical strength of the Al-Si-Cu film and was less thermally reactive than pure transition metals including Ti which increased the resistance after heat treatment [15]. The top TiN layer acts both as an antireflection coating layer for ultraviolet photolithography [17] and a buffer layer for counteracting the stress at the top corners of the Al-Si-Cu strip due to thermal expansion coefficient mismatch between Al-Si-Cu and the cover P-SiN.

Plane TEM micrographs of the Al-Si-Cu films for the corresponding structures, which were annealed at 500°C, are shown in Fig. 2(a)–(c), respectively. Average grain sizes of the structures were approximately 2, 0.7, and 0.4 μ m, respectively. It was found that the Al grain size in the Al-Si-Cu film, layered with the TiN/Ti film decreased in comparison with a single layer Al-Si-Cu on SiO₂ and that the Al grain size in the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti layered films further decreased.

X-ray diffraction analyses for the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer after annealing at 500°C are shown in Fig. 3. As-sputtered titanium nitride film was composed of tetragonal Ti₂N(200) as shown in Fig. 3(b). Ti(002) and Ti(101) were also observed in the TiN/Ti barrier layer. Al(111) was observed in the Al-1%Si-0.5%Cu on SiO₂ as shown in Fig. 3(a). After annealing, the tetragonal Ti₂N(200) changed to cubic

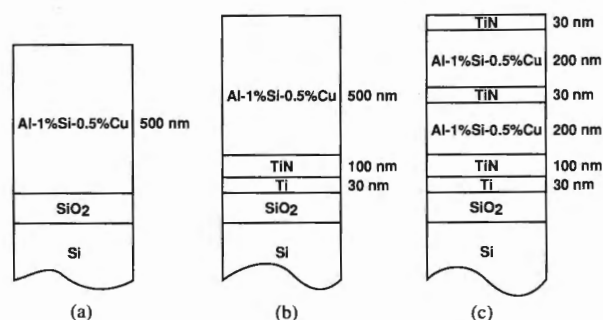


Fig. 1. Cross-sectional diagrams of (a) Al-Si-Cu single layer, (b) Al-Si-Cu on TiN/Ti barrier layer, and (c) TiN/Al-Si-Cu/TiN/Al-Si-Cu alternated layers on TiN/Ti barrier layer.

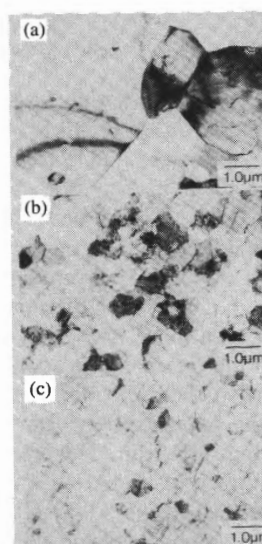


Fig. 2. TEM micrographs of Al-Si-Cu in (a) Al-Si-Cu single layer, (b) Al-Si-Cu/TiN/Ti, and (c) TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayers.

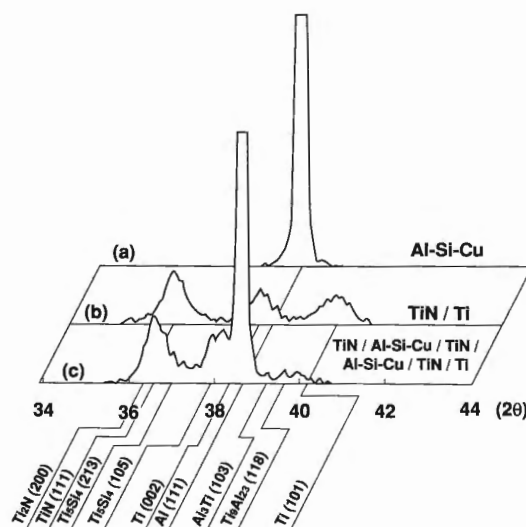


Fig. 3. X-ray diffraction analyses for (a) Al-Si-Cu, (b) TiN/Ti, and (c) annealed TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayers.

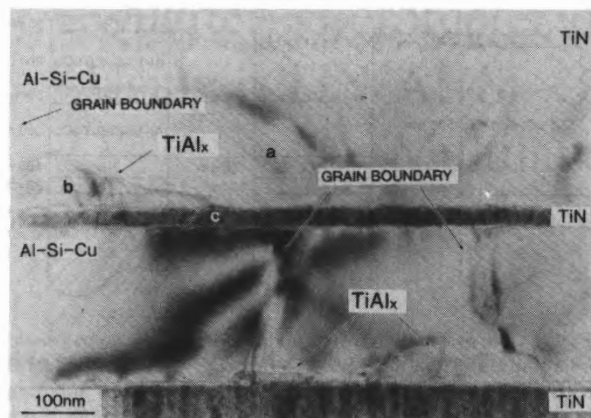


Fig. 4. A cross-sectional TEM micrograph for the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayers.

TiN(111) so that excess Ti atoms reacted with Al or Si atoms in the Al-1%Si-0.5%Cu film. As a result, intermetallic compounds such as TiAl_3 (103) and $\text{Ti}_9\text{Al}_{23}$ (118) were formed as shown in Fig. 3(c). Titanium silicides Ti_5Si_4 (213), (105) were also formed.

A cross-sectional TEM micrograph of the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti layered films is shown in Fig. 4. The grain boundaries in the upper Al-Si-Cu film were not aligned with those in the lower Al-Si-Cu film. It was found that the intermetallic compound precipitates were formed both at the grain boundaries of the Al-Si-Cu film and at the interface between the Al-Si-Cu film and the underlying TiN film. No precipitates were observed at the interface of the Al-Si-Cu and the overlaid TiN film. The surface of the Al-Si-Cu might have been passivated by an aluminum-nitride thin layer before and during the overlaid TiN reactive sputtering with N_2 and Ar gas mixture because N_2 gas was introduced in the vacuum chamber right after the Al-Si-Cu deposition.

The EDS analysis indicated that the intermetallic compound precipitates were composed of Ti, Al and Si as shown in Fig. 5(b). Fig. 5(a), (b) and (c) is a corresponding EDS analysis to the points *a*, *b*, and *c* in Fig. 4. It was consistent with the fact that the intermetallic compounds were identified by XRD as TiAl_3 and $\text{Ti}_9\text{Al}_{23}$. TiAl_xSi_y compounds may also be formed. Silicon was also observed in the TiN film as shown in Fig. 5(c). This is because of the reaction between Al-1%Si-0.5%Cu and Ti_2N and the formation of Ti_5Si_4 . An enlarged plane TEM micrograph, shown in Fig. 6, indicated that the intermetallic compound precipitates were formed at the triple junctions and along grain boundaries, corresponding to the cross-section TEM micrograph shown in Fig. 4. In addition, the resistivity increase of the multilayer after 500°C annealing for 1 h was approximately less than 10%. No significant resistivity increase was observed after 450°C annealing because the reaction of excess Ti and Si in the Al-Si-Cu could suppress the further formation of TiAl_x [15]. This result corresponds to the fact that the intermetallic compound precipitates were formed only at

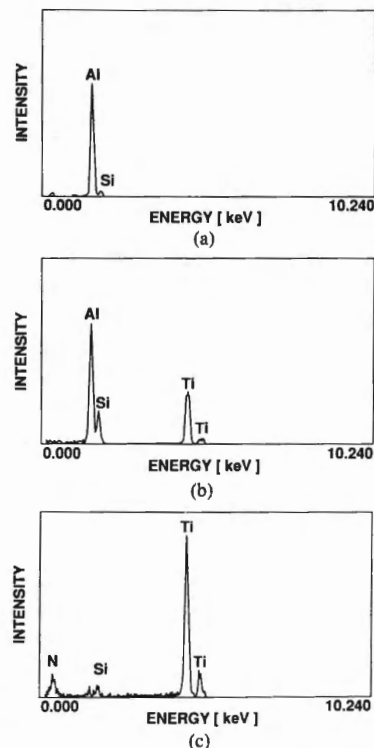


Fig. 5. EDS analyses for (a) the Al-Si-Cu, (b) the intermetallic compound precipitate, and (c) the TiN film, shown in Fig. 4.

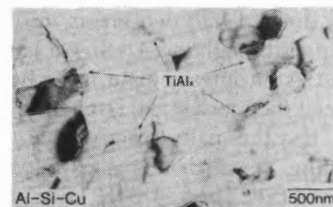


Fig. 6. A plane TEM micrograph for the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayers.

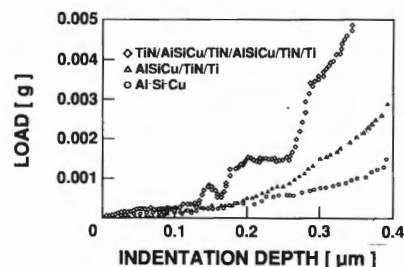


Fig. 7. Load versus indentation depth curves from the ultra-micro-indentation hardness measurements of Al-Si-Cu single layer, Al-Si-Cu/TiN/Ti, and TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayers.

the interface between the TiN and Al-Si-Cu and along grain boundaries, shown in Figs. 4 and 6.

Load versus indentation depth curves from the ultra-micro-hardness measurements for an Al-Si-Cu single layer on SiO_2 , an Al-Si-Cu single layer on TiN/Ti barrier layers, and TiN/Al-Si-Cu/TiN/Al-Si-Cu alternated layers on TiN/Ti barrier layers are shown in Fig. 7. Corresponding Vickers hardness values were 13, 19,

TABLE I
THERMAL AND MECHANICAL PROPERTIES OF MATERIALS

Material	Melting Point (°C)	Thermal Expansion Coefficient (1/°C)	Elastic Modulus ($E/1 - \nu$) (MPa)	Vickers Microhardness (10 MPa)	Reference
Al-Si-Cu	660	23.4×10^{-6}	1.02×10^5	12-14	[21], [22]
Ti	1660	8.5×10^{-6}	1.699×10^5	—	[22], [24]
TiN	2950	9.35×10^{-6}	5.87×10^5	1670-2050	[19], [25]
TiAl ₃	1340	10.65×10^{-6}	—	680	[19]-[21]
Si	1412	2.52×10^{-6}	1.81×10^5	—	[23]
SiO ₂	1600	0.5×10^{-6}	$0.63-1.64 \times 10^5$	—	[23], [26], [27]
P-SiN	—	2.48×10^{-6}	$1.1-3.7 \times 10^5$	—	[23], [26], [27]

and 31-53, respectively. It was found that the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer conductor was harder than the Al-Si-Cu single layer or the Al-Si-Cu on the TiN/Ti layers. This is because both TiN layer and intermetallic compound TiAl₃ have approximately 100 and 50 times larger Vickers hardness values than Al, respectively, as shown in Table I [19]-[27].

A SEM micrograph of a quarter-micrometer interconnection strip of TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti is shown in Fig. 8. After annealing at 450°C, neither surface hillocks nor lateral hillocks nor whiskers were observed for the multilayer conductors. This is due to the effect of the intermetallic compound formation both at the interface between TiN and Al-Si-Cu and at the triple junctions in the Al-Si-Cu, which could suppress grain growth and atomic migration of the Al-Si-Cu.

B. Stress-Induced Migration

Effective tensile stresses in a single Al-Si-Cu layer on SiO₂, a single Al-Si-Cu layer on TiN/Ti, and TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayers after heat cycles at 500°C are shown in Fig. 9. The effective stress for the layered film was defined as an overall residual stress against the Si substrate, which was calculated from the curvature of the Si substrate. The effective thickness of the overall layered film was defined as the sum of individual thickness for Al-Si-Cu, TiN, and Ti films. It was found that the Al-Si-Cu single layer showed residual tensile stress relaxation after heat cycles, while no residual tensile stress relaxation was observed for the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer structure after the first heat cycle. The Al-Si-Cu single layer formed both hillocks during heat treatment because of compressive stress relaxation, and voids or vacancies during cooling because of tensile stress relaxation. On the other hand, the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer structure could suppress both hillocks during heat treatment and voids during cooling. This is because the formation of rigid intermetallic compounds, TiAl₃, after the first heat cycle could suppress Al migration along grain boundaries and interfaces between TiN and Al-Si-Cu films.

Voids in the Al-Si-Cu strip and the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer strip after heat

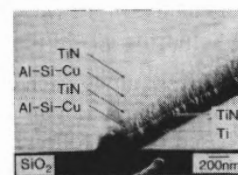


Fig. 8. A SEM micrograph of a quarter-micrometer wide TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer conductor strip.

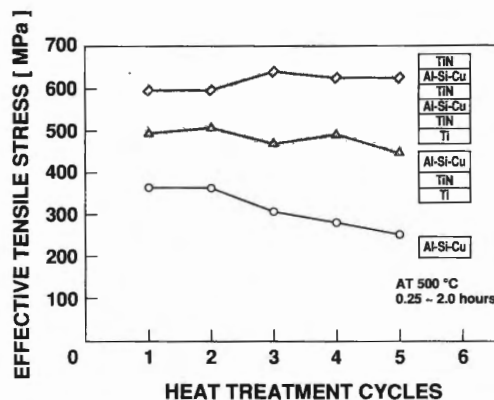


Fig. 9. Effective tensile stress change as a function of heat treatment cycles for an Al-Si-Cu single layer, as well as, Al-Si-Cu/TiN/Ti and TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayers.

treatment at 500°C, as a result of thermal and stress migrations, are shown in Fig 10(a) and (b), respectively. No void was observed in the multilayer strip, while a lot of voids were formed in the Al-Si-Cu single-layer strip. This result was consistent with the fact that no residual tensile stress relaxation occurred in the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer film after heat cycles as shown in Fig. 9.

Film stresses, due to thermal expansion coefficient mismatch between conductors and the Si substrate for a quarter-micrometer conductor strip covered with a P-SiN passivation film, were calculated from the finite-element modeling program called ANSYS [28]. The effective von Mises stress σ_{eff} is a scalar value based on all components of the stress tensor and proportional to the square root of the distortion energy of the material as shown in the fol-

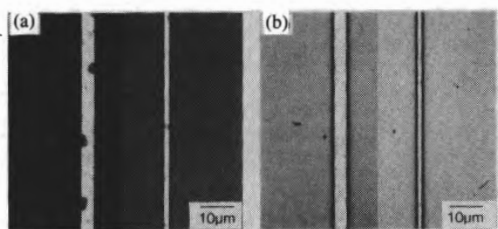
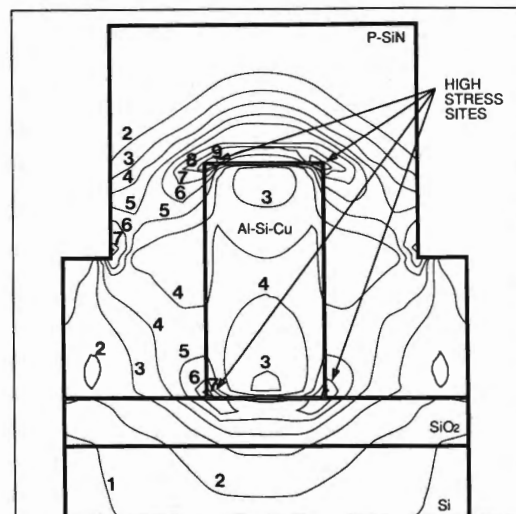


Fig. 10. Photomicrographs of (a) Al-Si-Cu single layer and (b) TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer conductor lines which are encapsulated with P-SiN films and annealed at 500°C.

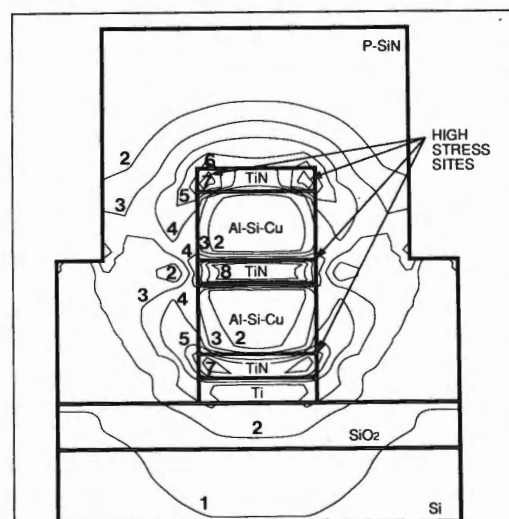
lowing equation [29]:

$$\sigma_{\text{eff}} = \frac{1}{\sqrt{2}} [(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)]^{1/2} \quad (1)$$

where σ is principal stress along each coordinate axis and τ is respective shear stress. The von Mises stress calculation, here, was based on the following assumptions: 1) only thermal stress was considered, 2) the thermal stress was zero during the P-SiN film deposition at 350°C and increased its tensile stress on cooling, 3) only elastic deformation was considered, and 4) intrinsic stress, as a result of film structure change due to thermal reaction, was not taken into consideration. Von Mises stress contour plots in the cross section of an Al-Si-Cu single-layer conductor strip and a TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer strip on cooling to 175°C are shown in Fig. 11(a) and (b), respectively. In the cross-sectional von Mises stress contour plots for Al-Si-Cu single-layer conductor strip which is covered with P-SiN film, the marked numbers 1, 2, 3, ... correspond to respective stress value started from 45 MPa (#1) in 73-MPa steps up to 629 MPa (#9). It is found that large von Mises stresses are generated at the top and bottom corners of the Al-Si-Cu single-layer conductor strip as shown in Fig. 11(a). The maximum stress in the Al-Si-Cu of the single-layer structure reaches 629 MPa if the stress relaxation does not occur. For TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer conductor strip, which is covered with P-SiN film, the numbers 1, 2, 3 ... correspond to respective stress values starting from 63 MPa (#1) in 106-MPa steps up to 805 MPa (#8), as shown in Fig. 11(b). The maximum stress is generated in the TiN layer. The resulting stress in the Al-Si-Cu layers of the multilayer structure is decreased to 487 MPa. This is because the thermal expansion coefficient of TiN is 9.35 ppm/°C [19], which is between those of Al (23.4 ppm/°C) [21] and Si (2.52 ppm/°C) [23] or P-SiN (2.48 ppm/°C) [23] and SiO₂ (0.5 ppm/°C) [23]. Furthermore, the elastic modulus of TiN is 5.87×10^5 MPa [25], which is five times larger than that of Al-Si-Cu, according to bulk data shown in Table I. Therefore, the maximum stress due to the thermal expansion coefficient mismatch between the multilayer and the P-SiN or Si or SiO₂ is generated in the TiN layers so that the stress of the Al-Si-Cu in the multilayer is decreased by the existence of the TiN. Although it is assumed in this calculation that the stress relaxation



(a)



(b)

Fig. 11. Cross-sectional von Mises stress contour plots. (a) Al-Si-Cu single-layer conductor strip covered with P-SiN film. (The contours marked 1, 2, 3, ... correspond to respective stress value starting from 45 MPa (#1) in 73-MPa steps up to 629 MPa (#9)). (b) TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer conductor strip covered with P-SiN film. (The contours marked 1, 2, 3 ... correspond to respective stress value starting from 63 MPa (#1) in 106-MPa steps up to 805 MPa (#8)).

does not occur and that the thermal expansion coefficient and Young's modulus of Al-Si-Cu are constant from room temperature to 350°C, relative comparison of the generated stress distributions between the single-layer and the multilayer metals would be meaningful.

C. Electromigration

Effects of annealing on the electromigration cumulative failure as a function of stress time for an Al-Si-Cu single-layer conductor and a TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti alternated-layer conductor are shown in Fig. 12. The electromigration test was carried out using current density 5×10^6 A/cm² at 242°C. The failure and

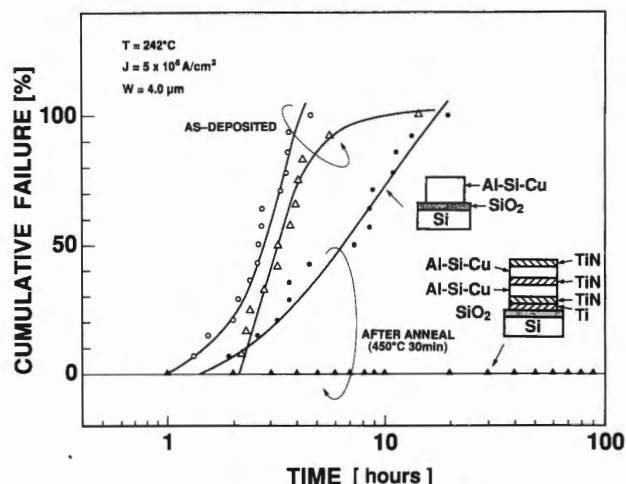


Fig. 12. Effect of annealing on the electromigration cumulative failure versus stress time for Al-Si-Cu single-layer and TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer conductors.

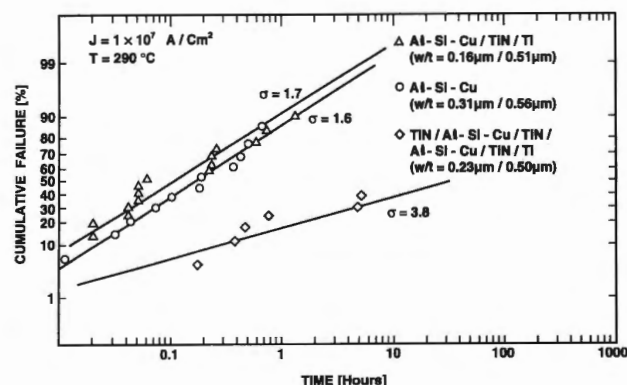


Fig. 13. Electromigration cumulative failure versus stress time for quarter-micrometer-wide Al-Si-Cu single-layer, as well as Al-Si-Cu/TiN/Ti and TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer conductors.

thus lifetime were defined when the metal line resistance increased 100% from its original value. Before annealing, no significant difference in terms of electromigration lifetimes was observed between the single-layer and the multilayer conductors. On the other hand, after annealing at 450°C, the multilayer conductor showed improvement of electromigration resistance in comparison with the single-layer conductor. This improvement in the electromigration resistance after annealing is due to the presence of rigid intermetallic compounds, $TiAl_x$, at the interface between the TiN and the Al-Si-Cu, and along grain boundaries of the Al-Si-Cu layer as shown in Figs. 4 and 6. The intermetallic compounds could suppress the electromigration of Al atoms. Fig. 13 shows electromigration cumulative failures versus time for various quarter-micrometer interconnections; Al-Si-Cu single layer, as well as Al-Si-Cu/TiN/Ti and TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer structures. The electromigration test was carried out at a current density 1×10^7 A/cm² and at 290°C. It should be noted that the

standard deviations of the log-normal failure distributions for quarter-micrometer-wide lines were very large because of the statistical uncertainty due to the deviation of each geometrical dimension of the metal line. Thus these results should be treated only qualitatively but not quantitatively. The mean time to failure of the TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer structure ($w = 0.23$ μ m) was 38 h ($\sigma = 3.8$), while those of the single-layer Al-Si-Cu ($w = 0.31$ μ m) and the Al-Si-Cu/TiN/Ti ($w = 0.16$ μ m) were 0.16 h ($\sigma = 1.6$) and 0.1 h ($\sigma = 1.7$), respectively. Since the standard deviation for the quarter-micrometer-wide multilayer strips was larger than those for Al-Si-Cu and Al-Si-Cu/TiN/Ti, the time to early failure (1%) may be equal although its mean time to failure was longer. The improvement in the mean time to failure may be attributed to the facts that 1) the quarter-micrometer-wide multilayer conductor strip had a bamboo structure in which the grain boundaries were strengthened by the rigid intermetallic compound, $TiAl_x$, and 2) the Al-Si-Cu conductor was divided into two layers, where each layer was strengthened by being sandwiched by the rigid TiN layers so that the probability of void propagation through the double Al-Si-Cu conductor layers became small. In addition, no lateral growth of whiskers was observed for the multilayer metal line after the electromigration tests. This would prevent short failure between the metal lines.

IV. CONCLUSION

A quarter-micrometer-wide TiN/Al-1%Si-0.5%Cu/TiN/Al-1%Si-0.5%Cu/TiN/Ti alternately layered conductor strip has been demonstrated to be a candidate for 256-Mb DRAM interconnections. The TiN/Al-Si-Cu/TiN/Al-Si-Cu/TiN/Ti multilayer structure, which was reinforced by both rigid TiN layers and $TiAl_x$ intermetallic compounds, had high electrical and mechanical durabilities in comparison with an Al-Si-Cu single layer or an Al-Si-Cu layered with TiN/Ti.

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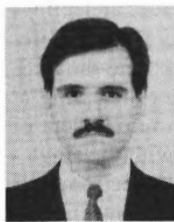
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