degradation prior to the initiation of electrical trees. Indeed, if the density of the injected electrons is sufficiently high, the existence of molten material observed in the vicinity of the breakdown region[13,14] might substantiate this scenario. However, it should be pointed out that the calculations at higher applied voltage including the space-charge effects and the more detailed electronic structure of SiO_2, as well as the nonpolar electron-phonon interactions, would be necessary to draw any conclusions.

In summary, we have performed the Monte Carlo calculations of the electron transport in SiO_2 subject to a strongly inhomogeneous electric field produced by a hyperboloid needle and plate assembly. A characteristic overheating due to the nonuniform high electric field near the needle tip has been observed.

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W_xN_{1-x} alloys as diffusion barriers between Al and Si

F. C. T. So,[a] E. Kolawa, X.-A. Zhao,[b] E. T-S. Pan, and M.-A. Nicolet
California Institute of Technology, Pasadena, California 91125

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Reactively sputtered tungsten nitride (W_xN_{1-x}) layers are investigated as diffusion barriers between Al overlayers and Si shallow n^+-p junctions. Both amorphous $W_{80}N_{20}$ and polycrystalline $W_{60}N_{40}$ films were found to be very effective in preserving the integrity of the n^+-p diodes for 30-min vacuum annealing up to 575 °C. Diode failure at higher temperatures is caused by localized penetration of Al into ⟨Si⟩ through the W_xN_{1-x} barriers. The effectiveness of the barrier decreases for polycrystalline $W_{90}N_{10}$ and is worse for pure W.

As device dimensions in integrated circuits are continuously scaled, it becomes essential for device reliability to incorporate diffusion barriers in contact structures to semiconductors. The high reactivity of refractory metals, such as Ti and W, with Al limits their use as diffusion barriers between Si and Al to post-metallization sintering below 450 °C.[1,2] For processing temperatures above 450 °C and long-term stability, nitrides of refractory metals are often favored as barrier materials.[3] Titanium nitride has been studied very extensively for barrier implementation in many process environments.[4,5] With the advent of low pressure chemical vapor deposition processes,[6] tungsten-based barrier materials are expected to play increasing roles in contact metallurgy. Since the presence of impurities (O, N, C) in refractory metal diffusion barriers has always been found to be beneficial in enhancing the stability of contact structures,[7] we consider here the simple case of nitrogen-doped W deposited by sputtering of tungsten in Ar-N_2 mixture.

Kattelus *et al.*[8] previously have shown by MeV He^+ backscattering spectrometry and sheet resistance measurements that reactively sputtered W_xN_{1-x} far surpass W as a diffusion barrier between Si and Al. In this work, the effectiveness of reactively sputtered W_xN_{1-x} barriers is evaluated by electrical measurements performed on shallow implanted n^+-p diodes with ⟨Si⟩/W_xN_{1-x}/Al contact structures, in addition to depth profiling analysis by backscattering. Shallow junction diodes are among the most sensitive devices to detect Al-Si interaction that occurs on a microscopic scale. Both polycrystalline and amorphous W_xN_{1-x} were deposited[8,9] and their performance as diffusion barriers is compared.

Our test vehicles consist of ⟨100⟩ Si n^+-p diodes of 0.35-μm junction depth formed by As^+ ion implantation (150 keV, 7×10^{15} As/cm^{-2}) and subsequent annealing. Details of the fabrication procedure have been reported elsewhere.[10]

[a] Present address: Optoelectronics Division, Hewlett-Packard Co., San Jose, CA 95131.
[b] Permanent address: Shanghai Institute of Metallurgy, Academy of Sciences of China, Shanghai, China.

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The size of the junction areas and contact windows are 500×500 and 300×300 μm^2, respectively. The W_xN_{1-x}/Al contact metallization was delineated by the lift-off technique.

Depositions of W_xN_{1-x} and Al were carried out in an rf sputtering system equipped with a diffusion pump and cryogenic baffle. The sputtering chamber was evacuated to a base pressure of 1×10^{-6} Torr before deposition. Tungsten nitride films were obtained by sputtering a 99.9% W target in premixed Ar and N_2 gas ambients. Three W_xN_{1-x} films were chosen for diffusion barrier tests: $W_{90}N_{10}$, $W_{80}N_{20}$, and $W_{60}N_{40}$. The sputtering parameters for obtaining these W_xN_{1-x} films have been described elsewhere.[11] Plain tungsten barriers sputter deposited in Ar were also examined for comparison. Following the W_xN_{1-x} deposition, Al overlayers of 5000 Å in thickness were deposited without breaking vacuum to complete the ⟨Si⟩/W_xN_{1-x}/Al contact structures. Such W_xN_{1-x}/Al layers were also deposited on unpatterned Si substrates and SiO_2 for depth profiling analysis by backscattering spectrometry. In these samples, the thickness of Al are in the range of 2800–3500 Å. The spot size of the analyzing beam was 1×2 mm^2.

$W_{90}N_{10}$ and $W_{60}N_{40}$ are polycrystalline and have resistivities of about 100 and 350 $\mu\Omega$ cm, respectively.[9,11] $W_{60}N_{40}$ consists predominantly of the W_2N phase while $W_{90}N_{10}$ is made up of a mixture of W and W with the nitrogen probably residing in the grain boundaries. On the other hand, as-deposited $W_{80}N_{20}$ films are x-ray amorphous by Read camera diffraction analysis and crystallize at 620 °C for a 30-min annealing duration. The resistivity of $W_{80}N_{20}$ is 200 cm. The amorphous barrier has the lowest compressive stress among the four film types considered here (1.5 GPa); the stress levels of the other three are comparable (4 GPa).

Annealing of the samples was carried out in a vacuum of better than 1×10^{-6} Torr in the temperature range of 350–600 °C. Unless otherwise stated, the annealing duration for each temperature cycle is 30 min. The reverse leakage currents of a set of 30–40 diodes were measured for every heat treatment.

Figure 1 shows backscattering spectra of ⟨Si⟩/$W_{80}N_{20}$/Al before and after annealing at 575 and 600 °C for 30 min. Very little interdiffusion between the adjoining layers can be detected up to annealing at 575 °C (Fig. 1). Heat treatment at 600 °C leads to a significant interaction between Al and the underlying $W_{80}N_{20}$ layer and ⟨Si⟩. This is evident from a partial disappearance of the Al plateau and the movement of the whole W signal towards the surface position in the BS spectrum. X-ray analysis, however, did not indicate the presence of any W-Al intermetallics in any of the annealed samples. This shows that failure of the ⟨Si⟩/$W_{80}N_{20}$/Al system cannot be attributed to the consumption of the $W_{80}N_{20}$ layer by Al to form WA_{12}, as in the case of a W/Al couple.[2] Also, no metallurgical interactions can be detected at 600 °C if ⟨Si⟩ is replaced by SiO_2. This shows that ⟨Si⟩ is involved in the reaction, most certainly by interacting with Al at 600 °C.

Histograms of the reverse leakage current distributions of the n^+-p diodes with the ⟨Si⟩/$W_{80}N_{20}$/Al contact structure after annealing at 350, 575, and 600 °C are shown in Fig. 2. The reverse currents remain narrowly distributed around 5×10^{-11} A (or 2×10^{-8} A/cm^2) at 550 °C. At 575 °C, about 10% of the diodes develop high leakage currents. (Diodes with reverse current densities higher than 8×10^{-8} A cm^{-2} are regarded as failure.) Even after a 600 °C sintering, about 70% of the diodes still survive despite backscattering analysis revealing barrier breakdown. This suggests that Al penetrates in a highly localized manner through the $W_{80}N_{20}$ layers and into the device junctions. Scanning electron microscopy inspection showed that the contact areas of diodes which survive the 600 °C treatment retain their smooth sur-

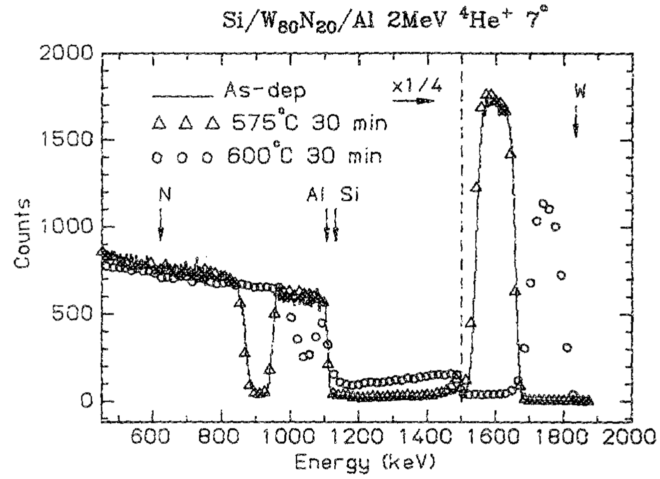

FIG. 1. 2 MeV $^4He^+$ backscattering spectra of a ⟨Si⟩/$W_{80}N_{20}$ (800 Å)/Al(3400 Å) sample before and after annealing at 575 or 600 °C for 30 min. The detected particles are scattered by an angle of 170 °; the angle between the incident beam and the sample normal is 7°.

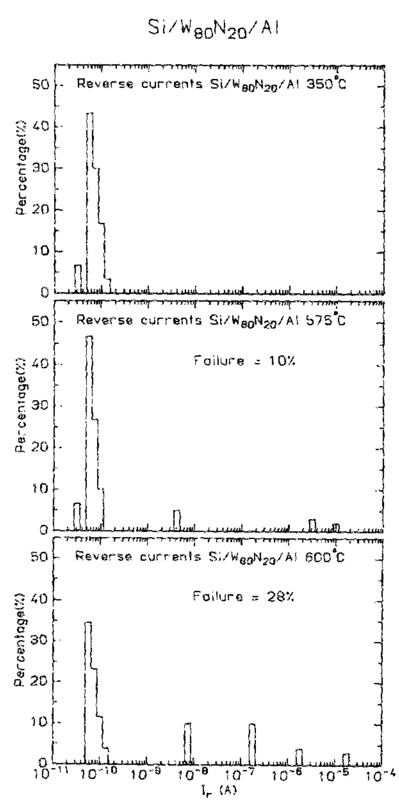

FIG. 2. Histograms of reverse current distributions of Si n^+-p diodes with ⟨Si⟩/$W_{80}N_{20}$/Al contacts annealed at 350, 575, and 600 °C for 30 min.

face morphologies. In contrast, one or two square pits are easily visible in the contact region of a shorted diode. The presence of pits with the symmetry of the ⟨100⟩ Si substrate proves that contact was established between the Al overlayer and the ⟨100⟩ Si substrate through localized weak spots or defects in the $W_{80}N_{20}$ layers covering the contact holes. Surrounding the square pits are droplets of obviously resolidified material. They must arise from Si-Al melting. The Al-Si binary system has a eutectic point at 577 °C. It evidently must be the existence of this eutectic that underlies the rapid deterioration of the contact scheme above that temperature.

Similar results were obtained with polycrystalline $W_{60}N_{40}$ barrier layers. Extremely low diode failure rates were found up to annealing at 575 °C. A 600 °C thermal cycle caused ~52% of the measured diodes to fail, which slightly exceeds that of amorphous $W_{80}N_{20}$ barriers. Backscattering and SEM analysis suggest that the failure mechanisms in both cases are alike. Diodes with $W_{80}N_{20}$ or the $W_{60}N_{40}$ barrier layers in their contact structures were also subjected to extended heat treatments at 500 °C for 13 h to simulate the worst case processing exposure.[12] The failure rate was by a factor of 2 lower for amorphous $W_{80}N_{20}$ (23%) than for $W_{60}N_{40}$ (46%) barriers.

Failure mechanisms of these contact systems at 500 °C may be quite different than those which dominate above the Al-Si eutectic temperature. This failure mode is examined here.

The polycrystalline $W_{90}N_{10}$ film is inferior as a barrier to $W_{80}N_{20}$ or $W_{60}N_{40}$. A reaction between Al and $W_{90}N_{10}$ leading to the formation of WAl_{12} system can be detected at 550 °C by backscattering and x-ray analysis. Accordingly, all the diodes with ⟨Si⟩/$W_{90}N_{10}$/Al contacts were shorted after a 550 °C anneal. This observation implies that a W_xN_{1-x} barrier must contain enough nitrogen in the films in order to function effectively as a barrier between Al and Si at 550 °C and above. The plain W barriers fail metallurgically at 500 °C as a result of the consumption of W by Al, in agreement with previous work.[2] However, all the diodes with a W barrier layer were electrically shorted after annealing at 450 °C. This failure at 450 °C is probably caused by grain boundary diffusion of Al or Si through the W barrier that goes undetected by backscattering analysis. Pure W has long been advocated in the past as an effective diffusion barrier. That it should be so is an anomaly because pure elemental films do not, in general, make good diffusion barriers.[13] The present results suggest that W is not an exception to that rule. Rather, W films are difficult to produce in pure form which explains both its reputation as a good barrier and a debatable case. The percentage of diode failures as a function of annealing temperature (30 min) for the four barriers is summarized in Fig. 3.

Both amorphous and polycrystalline W_xN_{1-x} are far superior to W in suppressing Si-Al interaction up to 575 °C annealing for 30 min, provided enough nitrogen is present in the barrier films. Since the failure of ⟨Si⟩/W_xN_{1-x}/Al contacts at 600 °C is dominated by localized defects or pinholes in the W_xN_{1-x} barriers, contact hole size may have a significant effect on the performance of the barriers. The contact resistivities between W_xN_{1-x} and ⟨Si⟩ also deserve some future attention. In advanced contact structures, an appropriate silicide contacting layer will be inserted between the W_xN_{1-x} diffusion barrier, to ensure acceptable contact resistivities for ohmic contacts, or Schottky barrier heights for rectifying contacts.

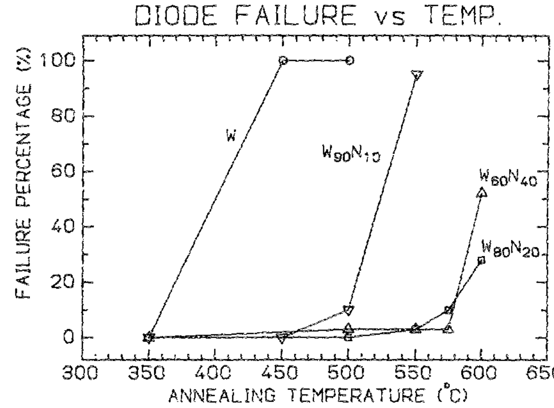

FIG. 3. Percentage of diode failure with ⟨Si⟩/W_xN_{1-x}(W)/Al contacts as a function of vacuum annealing temperature for 30 min.

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