PVD Processes in High Aspect Ratio Features by HIPIMS

J. Weichart and M. Elghazzali, OC Oerlikon Balzers Limited, Balzers, Liechtenstein;
S. Kadlec, Staccato Consulting, Praha, Czech Republic; and
A.P. Ehiasarian, Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, United Kingdom

ABSTRACT

High Power Impulse Magnetron Sputtering (HIPIMS) has been developed on rotating PVD magnetron sources for uniform deposition on 200mm single wafer tools for barrier and seed layer deposition in through silicon vias (TSV). The ionization degree has been analyzed by atomic absorption spectroscopy. Processes and hardware have been developed for HIPIMS of Ti, Ta and Cu with reasonable deposition rates and a high transfer factor due to low target substrate distance, good uniformities and low stress for the application in deep silicon etched features with very high aspect ratio (AR). For Ti a bottom coverage of 20% in trenches with AR 10:1 and 7% in trenches with AR 30:1 have been achieved. Studies with AR 10:1 vias have shown that continuous layers of Ti and Cu could be deposited inside the feature.

INTRODUCTION

In recent years, vertical interconnects in microelectronic chip stacks have been developed using Through Silicon Vias (TSV) as an alternative technology to wire bonding providing size reduction, improvement of the electrical performance and enabling heterogeneous integration [1-4]. TSV technology involves Deep Silicon Etching (DSE) [1,5] or laser drilling for creating via-holes in silicon substrates, via passivation, e.g. by PECVD SiO_2 or silicon nitride, barrier and adhesion layer deposition (Ti or Ta) and the deposition of a Cu seed layer for subsequent via filling. Cu is the preferred metal for through-wafer interconnects due to its low resistivity and desirable electromigration characteristics. Copper interconnects are deposited by sputtering a thin seed layer onto a barrier metal film (e.g., Ta-Cu or Ti-Cu) followed by electroplating. While some applications are already moving to volume production, there are still many open questions, like what aspect ratio (AR) vias will be required and what materials and techniques will be able to fill them. In via structures with AR > 3:1, it is required to deposit these layers by directional sputtering techniques to ensure a continuous layer in the entire via to enable electroplating. Directional sputtering is achieved through narrowing the angular distribution by a) long distance sputtering b) collimators [6] or c) ionization of the sputtered material. These methods are typically used in combination with a radio frequency (RF) induced self bias voltage applied on the substrate in order to remove overhanging materials from the features as well as to accelerate ionized metal to the substrate [7]. Ionized physical vapour deposition (IPVD) has been introduced in the 1990s to cope with the requirement of directional deposition in VLSI features with high AR. In most cases, the neutral metal vapour is ionized by additional excitation such as an inductive RF coil [8].

As a novel IPVD technology High Power Impulse Magnetron Sputtering (HIPIMS) or High Power Pulsed Magnetron Sputtering (HPPMS) has been introduced by Kouznetsov [9] using very short pulses of typically less than 0.2ms, a low duty cycle of less than 10% and high currents of several hundreds up to more than 1000 A or current densities up to 4 Acm^{-2} in the pulse as calculated by the peak current divided by the target area. In these discharges the target material is sputtered and subsequently ionized due to high plasma densities [10-13]. Plasma measurements indicate a peak electron density of the order of $10^{19}m^{-3}$, expanding from the target with a fixed velocity that depends on the gas pressure. The high electron density results in a high degree of ionization of the sputtered material. The ionization degree for HIPIMS near the target has been analyzed by optical emission spectroscopy and reported to be more than 90% for Ti [14]. A comparison with post-ionization by a RF coil showed that HIPIMS generates a twofold higher ionization degree which is constant over the distance, whereas the ionization by RF coil can only be found at distances greater than 10cm from the target [15]. The metal ionization degree and metal ion-to-gas ion ratios in HIPIMS depend strongly on the discharge current and can be adjusted in a wide range. The average energy of metal ions is of the order of 3-6eV, however when HIPIMS is operated at low pressure of 10^{-3} mbar, the high energy tail of ions can reach several 10s of eV near the substrate. The origin of the ion energy is mainly from the atoms generated during the sputtering process which are subsequently ionized in the plasma. The energy can be reduced by increasing the pressure [16].

EXPERIMENTAL SETUP AND CHARACTERIZATION METHODS

Deposition tools

For the development of the TSV barrier/seed layer deposition on 200mm wafers an industrial size PVD magnetron source with rotating magnet is used. This source called ARQ151 from Oerlikon Balzers Ltd. takes up a target diameter of 300mm directly cooled and specified for an

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average power up to 20kW. In a first phase this sputter source has been installed on a versatile lab tool enabling deposition runs on small test samples as well as running atomic absorption spectroscopy (AAS) for the characterization of the ionization degree. In the next step two of these ARQ151 sources were installed on a fully automatic cluster tool for single wafer (static) deposition; the Clusterline200-II production tool from Oerlikon. One of the sources was equipped with a Ti target and the other with a Cu target to allow subsequent deposition of Ti/Cu layers without vacuum breakage or time delay. Prior to the deposition an ICP sputter etch station was utilized to pre-clean the substrates. Both PVD modules were cryo-pumped and equipped with a substrate stage with mechanical clamping which allows substrate cooling by backside gas application. For the Cu station additionally a chiller is used to avoid segregation of Cu when thicker layers are deposited. On the substrate stage an RF bias together with a proper matching circuit is applied to accelerate the generated ions. The PVD discharge area is defined by removable stainless steel shields with a pumping labyrinth. The target substrate distance is adjustable by movement of the substrate stage between 50 and 80mm with appropriate shield sets.

HIPIMS plasma generation

For the generation of HIPIMS discharges, a power supply HMP-2/3 from Huettinger Elektronic Sp. z o.o. has been used. It consists of a DC charging unit, a capacitor bank and a computer controlled pulsing unit allowing peak voltages up to 2000 Volts and peak currents up to 3000 Amps, hence a maximum peak power up to 6MW. The pulse length is adjustable between 1 and 200µsec and the pulse repetition rate is adjustable between 1 and 500Hz. The DC unit allows an average power of up to 20kW.

Atomic absorption spectroscopy (AAS)

The ionization degree of the metal vapour sputtered by HIPIMS from the sputter source ARQ151 has been evaluated on the lab tool by AAS described elsewhere [13]. In the experimental setup a parallel light beam with a wavelength characteristic for the Ti^0 and Ti^{1+} species passes through the sputtered Ti vapour. The light is absorbed by a value that corresponds to the density of each species. This allows quantifying the Ti^{1+} / (Ti^{1+} + Ti^0) ratio and thus providing a first approximation of the ionisation degree. As a light source a hollow cathode lamp operating in giant pulse mode is used and the selected lines are chosen to be transitions to the ground state for neutral metal as well as for metal ions. The sputtered vapour had to be thermalized to avoid Doppler effects and therefore the Ar gas pressure in the chamber was increased to $2x10^{-2}$ mbar. AAS was performed at a distance of 130mm from the target surface, which is significantly further away from the target than the typical target substrate distance (50 to 80mm) used in the processes as described above.

Deep silicon etch (DSE) technology

To produce wafers with vertical sidewall features of AR up to 30:1 in silicon DSE technology has been applied on a Versaline tool by Oerlikon. This so called “Bosch” process is using a series of alternating isotropic etch and anisotropic steps with deposition of sidewall passivation [1,5]. Depending on the duration of the alternating etch steps, the “Bosch” process generates more or less scallops in the feature sidewalls. Since a high roughness especially in the undercut areas of the scallops inhibits a continuous deposition a trade-off between the sidewall roughness and the silicon etch rate has to be found. By using step times of 0.5 to 1.0 seconds a sidewall roughness of 50 to 100nm could be achieved at an etch rate in the range of 7-8µm/min. Features with mainly trenches were produced on the DSE etcher since trenches are preferred during the optimization phase for ease of preparation by simple wafer breakage and inspection of the cross section by scanning electron microscopy (SEM). In most of the experiments sample pieces of approx. $14x14mm^2$ with trenches of AR ranging from 2:1, 6:1, 10:1 and 30:1 with trench depth between 60 and 100µm were placed on a carrier wafer, which is transported through the tool.

Film characterization

Thickness measurements were performed by a Veeco step profiler on steps of the deposited film produced by lift off or etching technique. Resistance measurements were done by a 4-point-probe resistivity mapper from Four Dimension Model 280 TCI. Scanning electron microscopy (SEM) as well as Focussed Ion Beam (FIB) SEM (Zeiss 1540 XBeam) were performed to evaluate the film distribution in trenches and vias. For via analysis the wafers were broken along a line with many vias and the cross section was polished by FIB and subsequently analyzed by SEM. For vias with a dual layer of Ti/Cu inside also Energy Dispersive X-ray Spectroscopy (EDX) was used to quantify the materials along the walls.

Monte Carlo simulation of the deposition profile in vias and trenches

For the practice of process development it is required to provide a tool for the comparison and prediction of these profiles in vias and trenches with different AR and profiles. Here the Monte Carlo code SIMBAD 2.1.4 has been applied [17,18]. This code calculates the angular distributions for neutral metal and ionized metal for given chamber and substrate diameter, target-substrate-distance, target erosion profile, gas mass and pressure, as well as target material data (mass, binding energy and collision cross-sections). In the second stage these angular distributions are used together with assumptions for the ionization degree, Argon ionization and their angular spread, sticking and re-sputtering coefficients for both ions and neutral atoms to calculate the deposition profile in the feature. In practice for example the results of HIPIMS were measured in trenches for ease of preparation simply by cleaving the silicon wafer piece perpendicular to the trench direction. DSE trenches with different AR on the same wafer piece are considered and the results are compared with simulation profiles in trenches calculated for different parameter settings. Once a parameter setting gives reasonable results it is applied for vias with different ARs and shapes to predict their coverage, since the preparation of vias is much more difficult than for trenches. The difficulty is that there is still very little understanding of the highly transient HIPIMS process. The SIMBAD code is written for IPVD application but it is not able to take pulsed processing into account. Most of the simulation parameters are only roughly known, especially since re-sputtering inside the feature has to be considered to obtain a proper simulation of the deposition profile.

RESULTS AND DISCUSSION

The ionization degree was evaluated in the lab tool for a HIPIMS discharge of Ti with rotating target by AAS in a distance of 13cm from the target. The measurements were captured as function of the HIPIMS peak current at a delay time of 500µsec after the HIPIMS voltage was switched off. In Figure 1 the results of the AAS measurements are plotted showing that the absorption of Ti^{1+} is steadily increasing with increasing peak current whereas the Ti^0 reaches a maximum and starts to decrease above 600A. The ionization degree calculated from these two absorption signal shows that it reaches a value of 46% at a peak current of 1000A.

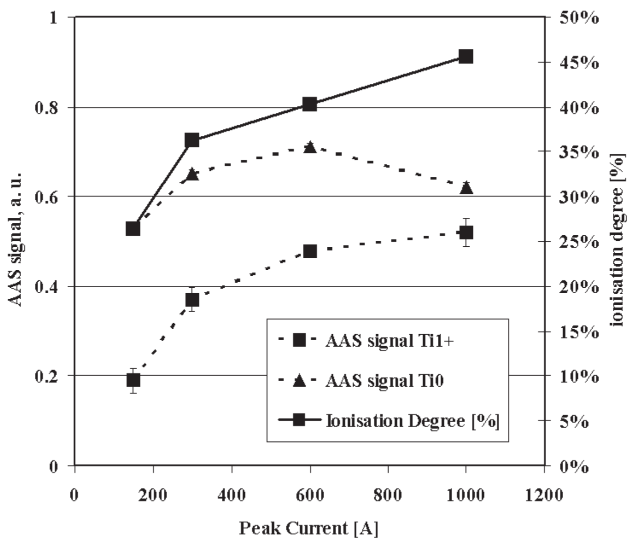

Figure 1: AAS signals and ionization degree for HIPIMS Ti.

Additional results achieved on the versatile lab tool have been published elsewhere [19]. In the following the HIPIMS process has been transferred on the Clusterline200 and applied on the Ti chamber with, for the first experiments, a magnet system which has been developed for regular DC sputtering at a target distance of 50mm. A significant reduction in the specific deposition rate, defined as the deposition rate divided by the average power, is being observed. The rate is decreasing further with increasing peak power, given by the product of the peak current and the voltage, as plotted in Figure 2. At the same time the film thickness is developing towards less uniform films with increasing peak power.

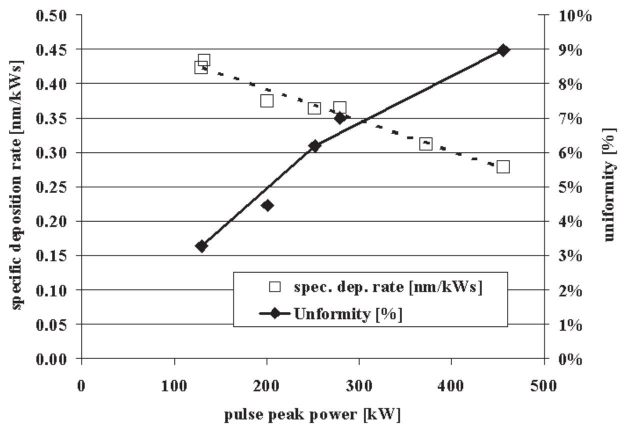

Figure 2: Deposition rate and uniformity for HIPIMS Ti as function of the pulse peak power.

Figure 3 shows the normalized shape of the deposition profile across a Si wafer of 200mm diameter for different pulse peak powers. The rotating magnet set used in this experiment has been optimized to give a flat deposition profile for Ti with regular DC sputtering. It is generally observed that the deposition profile is increasingly dome shaped with higher peak currents. One possible explanation for this effect is that the magnetic field is attenuated by the opposed magnetic field generated by the high drift current. In [20] it has been shown that the drift current of the HIPIMS discharge is a factor of 2 higher than the current to the cathode. Another explanation is that the positive ions follow ambipolar diffusion towards the chamber walls resulting in a radial metal ion gradient being higher than the gradient of the neutral metal. The change of the deposition profile has to be compensated by a proper design of the magnet which is principally no issue; however it should be noted that processes with different peak currents in the same chamber will require different magnet sets. Also the rate drop for HIPIMS does not mean a disqualification for TSV applications since here the deposition rate inside deep features is actually enhanced. Taking these effects into consideration, processes for Ti, Ta and Cu have been optimized with respect to deposition rate, specific resistivity, uniformity and film stress. The results are summarized in Table 1. The specific resistivity is slightly higher than typical bulk value due to a fine-grained microstructure of the films. Please note that α-phase Ta could be obtained with an extremely thin seed layer due to high ionization.

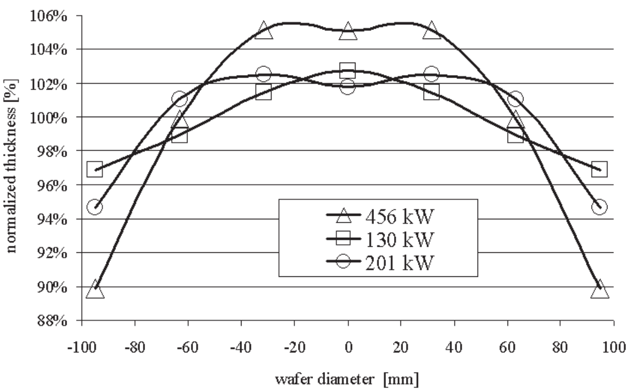

Figure 3: Uniformity profile for HIPIMS Ti as function of the pulse peak power.

These HIPIMS processes are applied on DSE trenches and the trenches are cleaved and analyzed by cross section SEM. Figure 4 shows the positions analyzed in the trench. In Figure 5 the deposition profile in trenches of AR 10:1 and 30:1 are plotted for samples taken from the wafer centre as well as from the wafer edge. With the latter it can be demonstrated that there is no geometrical effect visible for these high AR and therefore that the directional deposition is completely driven by the RF self bias field applied to the substrate. As can be seen in Figure 5 the bottom coverage in the 10:1 trench is 20% and in the 30:1 trench still 7% Ti can be found. However the more critical positions are the bottom edge and the lower sidewall.

Similar test were performed for Cu and Ta showing that these materials typically provide roughly half of the bottom coverage of Ti. Besides some lower ionization it is assumed the higher mass of Cu and Ta results in less thermalization and therefore a broader angular distribution with respect to Ti.

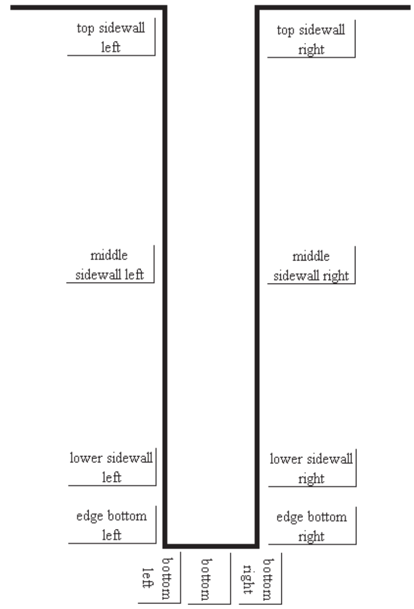

Figure 4: Measurement positions in a DSE trench.

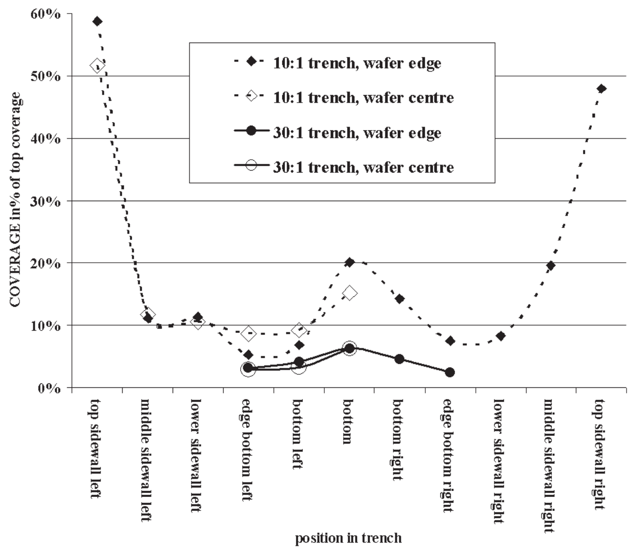

Figure 5: Deposition profile for Ti deposited in a DSE trench with AR 10:1.

Table 1: Film properties for HIPIMS processes.

Material	Deposition Rate	Specific Resistivity	Uniformity, 1/2 range/mean		Film stress
	[nm/s]	[μΩcm]	on 150mm	on 200mm	[MPa]
Ti	2.8	70	± 1.3%	± 6%	-560
Ta (α-phase)	3.2	26	-	± 6%	-700
Cu	6.6	2.7	± 5.7%	± 6%	160

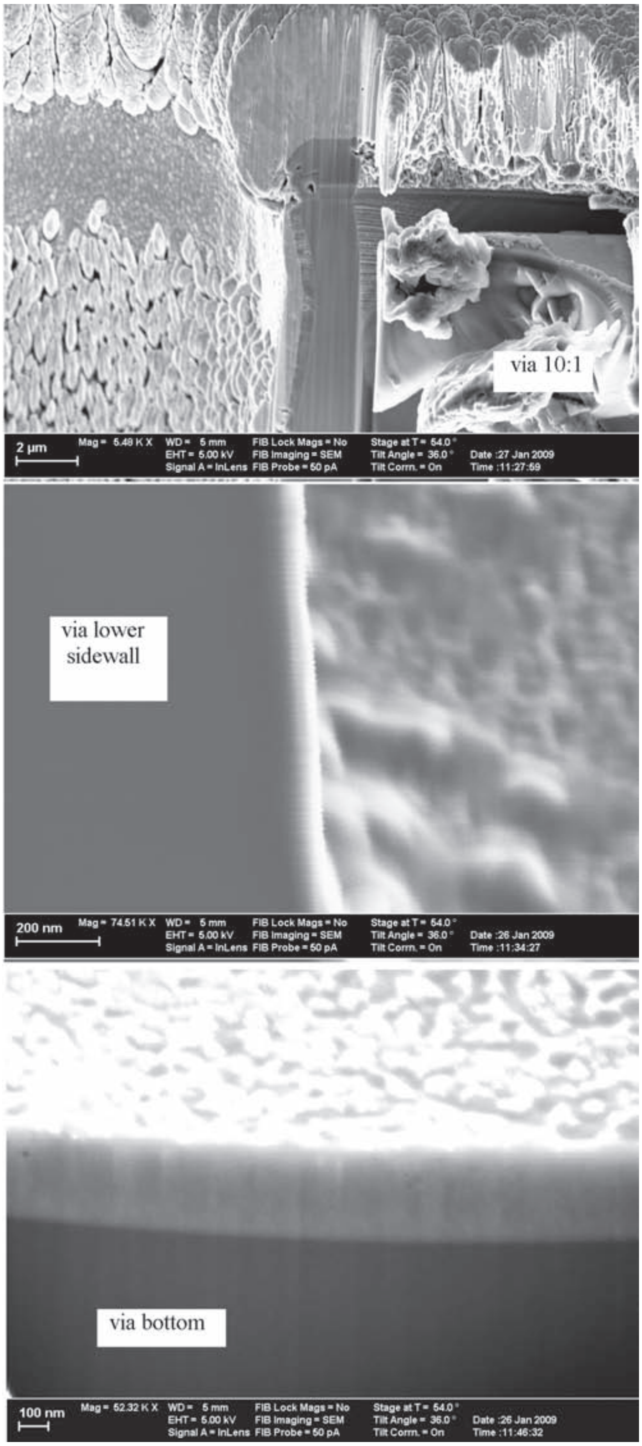

Figure 6: FIB SEM pictures of Ti/Cu layers in a via with AR 10:1.

The process was applied to vias of 100µm depth with AR 10:1 where relatively thick layers of Ti (1.5µm) and Cu (4µm) were deposited in order to get reliable thickness data. It should be mentioned that barrier/seed layers will be applied to approx. half of this thickness in production. Figure 6 shows FIB SEM cross sections of these vias from the top, the lower sidewall and the bottom. There is still more than 300nm material in the bottom and a minimum of 40nm along the sidewalls. The SEM analysis did not allow distinguishing between the Cu and the Ti layer, but it was possible to detect Cu all along the sidewall by EDX. By comparing the EDX Cu L signal with positions where the thickness was known it was tried to generate a profile for both materials. The result is plotted in Figure 7. Please note that the mid side wall thickness is lower than the lower sidewall coverage measured near the bottom edge. This effect is due to re-sputtering of material from the vias bottom as could be confirmed by Monte Carlo simulation (SIMBAD).

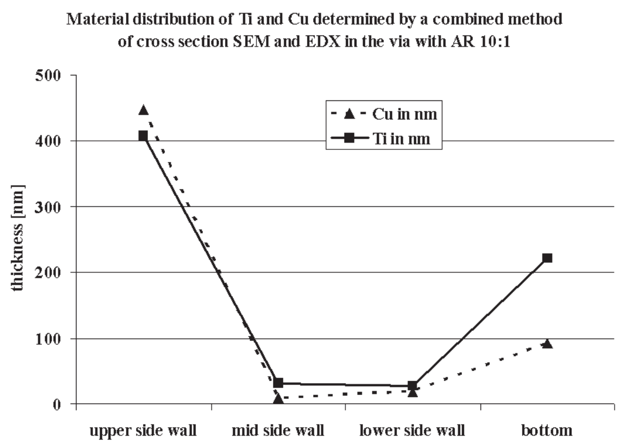

Figure 7: Material distribution of Ti and Cu determined by a combined method of cross section SEM and EDX in the via with AR 10:1.

CONCLUSIONS

HIPIMS has been applied on rotating PVD magnetron sources for uniform deposition on 200mm single wafer tools for through silicon via (TSV) metallization in 3-dimensional Packaging. The big advantage of HIPIMS is that the technology can be applied to regular PVD sources working at low target to substrate distance of typically 5cm; by this providing a high transfer factor and a cost-effective process for directional sputtering. However 10 to 40% rate loss and uniformity depending on the value of ionization current have to be taken into account.

The ionization degree of Ti has been determined by AAS to be 46% in a distance of 13cm from the target. Processes have been optimized for Ti, Ta and Cu with RF bias applied on the substrate to accelerate the generated ions into deep silicon etched trenches and vias of very high aspect ratio (AR) up to 30:1 with vertical sidewalls. For Ti a bottom coverage of 20% in trenches with AR 10:1 and still 7% in trenches with AR 30:1 have been achieved at a deposition rate of 28Å/s. It is more difficult to direct Cu into deep features, however Ti and Cu deposited in a combined process could be found at reasonable thickness all along in 10:1 vias, thus allowing electroplating of the vias as a subsequent step.

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