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Modeling of Electromigration Induced Contact Resistance Reduction of Cu-Cu Bonded Interface.

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Metal to metal bonding, particularly Cu-Cu bonding, is an important part of three dimensional integrated circuits (3DICs) that utilizes wafer bonding. The use of Cu to Cu bonding in 3DICs is advantageous as it functions as both the glue layer and electrical interconnection. It has been observed that the contact resistance of bonded Cu interface could be decreased under direct current stressing. In this paper, the mentioned phenomenon is modeled and simulated. Electromigration induced contact resistance reduction of bonded interconnects may provide a method for post-bonding bond property improvement for 3DICs.

Introduction

Continued scaling of integrated circuit (IC) devices according to Moore’s Law has presented challenges in interconnection, such as long wiring, power consumption, signal delay, etc. Three dimensional integrated circuits (3DICs) has been proposed as a possible solution to some of the challenges. 3DIC represents a generic technology and process that utilizes the third dimension of electronic circuits to connect different chips and functionalities. The utilization of the third dimension introduces the possibility of shorter wiring, lower interconnection resistance, shorter signal propagation delay, reduction in power consumption and possibility of heterogeneous device integration.

3DIC can be realized through 3D-IC packaging, 3D-monolithic integration, wafer level or chip level 3D-IC stacking with through substrate via. 3D-Monolithic Integration builds active semiconductor device layers sequentially up on the first IC layer (1). Meanwhile, in 3DIC stacking, individual wafers are first fabricated and then stacked vertically with through-Si vias (TSV) which provide the interconnections between dice. This technology option is gaining in popularity due to its ability to provide optimal functionality/volume and relatively low-cost heterogeneous integration of diverse technologies. IC-stacking can either be done at wafer-level or at die-level (2). 3DIC stacking process includes wafer or chip bonding and alignment, fabrication of TSV and wafer thinning (3).

Recently, direct Cu bonding (4) and Cu thermocompression bonding (5-8) are seen as a general route to realize 3DIC with bonded metals providing both mechanical adhesion as well as electrical interconnection. Wafer bonder’s high cost of ownership and low wafer output has driven two stages of bonding process, i.e. thermocompression bonding followed by thermal annealing (8, 9). The two stages process enables short
thermocompression bonding which increases the wafers output, while the post-bond thermal annealing enhanced the bond interface which can be done as a batch processing. Furthermore, Chen et. al. (10) and Leong et. al. (11) have observed that the contact resistance of bonded Cu interface can decrease under direct current stressing. As a lower contact resistance implies better mechanical bond integrity, contact resistance reduction by current stressing opens up a new method for post-bonding Cu bond interface enhancement. Chen et. al. (10) reported that irreversible resistance reduction was observed when the current was ramped from 1 mA to 100 mA as shown in Figure 1(a). A commentary paper by Timsit (12) suggested that the true contact area could be small enough that will allow electromigration to occur even at room temperature. Furthermore, elevated temperatures around the interface could also enhance this effect. Leong et. al. in (11) observed that the resistance reduction only started to appear when the current stress level had reached a certain value. Furthermore, it was also reported that this threshold current is higher for smaller initial resistance. Whereby, beyond the critical current, the contact resistance starts to drop exponentially (10). In this paper, bond strength enhancement through current stressing is modeled and comparison between the simulation and published experiments is discussed.

![Figure 1](image_url) Contact resistance reduction under current stressing, (a) reproduced from Chen et. al. (10) and (b) extracted from Leong et.al. (11).

### Dependence of Contact Resistance on True Contact Area

As a consequence of surface's micro roughness, contact of nominally flat surface can be consisting of multiple spots (13) and voids. The contact area covers only certain discrete areas and not the whole nominal contact area, and hence is commonly referred to as the true contact area (14). The ratio of the true-to-nominal contact area can be a very small value and can be a link between adhesion and electrical contact resistance (15).

The total true contact area $A_c$ between nominally flat surfaces but microscopically rough surfaces can be calculated based on a method elaborated by Greenwood and Williamson (GW) (14). GW formulated that when large flat surfaces are pressed together, their mean planes become parallel. Contact of two rough surfaces can be modeled as contact of an equivalent rough surface to a perfectly flat plane as shown in Figure 2.
Figure 2. Schematic of multispot contact area. If a rough surface and a smooth surface are pressed against each other until the summit mean plane of the rough surface and the mean plane of the smooth surface are separated by an amount of $d$, summits that have a height $z > d$ will deform.

If the rough and smooth surfaces are pressed against each other until the summit mean plane of the rough surface and the mean plane of the smooth surface are separated by an amount of $d$, summits that have height $z > d$ will deform. In randomly distributed summits, the total number of deformed asperities that form micro contacts is (16)

$$N_i = A_n \eta \int_{dz}^{\infty} f(z)dz,$$  \hspace{1cm} \text{(1)}$$

where $A_n$ is the nominal contact area, $\eta$ is the asperity density per unit area and $f(z)$ is the asperity height distribution function. Contact radius of each contacting asperity had been shown to be (6)

$$a_i = \sqrt{2R_i(z_i - d)},$$  \hspace{1cm} \text{(2)}$$

where $R$ is the radius of curvature of the asperity and $z$ is the asperity height. Whereas the total true contact area is given by (16)

$$A_c = \int_{dz}^{\infty} \eta A_n \pi R(z - d)f(z)dz,$$  \hspace{1cm} \text{(3)}$$

where $\overline{R}$ is the average of the asperity tips curvature radius.
Theoretical estimate of the contact resistance $R_c$ for Cu-Cu bonded interface had been conducted by Leong et. al. (5) Contacting spots can be considered as a linear resistor connected in parallel. Electrical contact resistance of each contacting asperity can be expressed as (21, 22)

$$R_{ci} = \Gamma(l/a_i) \left( \frac{\rho}{2a_i} \right) + \frac{4\rho l}{(3\pi a_i)^2}$$

[4]

where $l/a_i$ is the Knudsen ratio, $l$ is the electron mean free path, $a_i$ is the contact radius, $\Gamma(l/a_i)$ is a function that has value decreasing from 1 to 0.694 as $l/a_i$ increases from 0 to $\infty$, (19) and $\rho$ is the material resistivity. Individual radius of contacting asperity $a_i$, can be calculated based on [2].

With the number of contacting asperity $N_i$ calculated (16), an equivalent resistance $R_c$ for the entire contacting surface then simply can be calculated as

$$\frac{1}{R_c} = \sum_{i=1}^{N_i} \left( \frac{1}{R_{ci}} \right)$$

[5]

**Modeling of Contact Resistance Reduction Under Current Stressing**

Since 1969, electromigration has been considered as the interconnect enemy (20, 21). Until recently, electromigration remains a dominant reliability concern for the modern IC, due to the aggressive decrease in interconnect dimensions and the comparably aggressive increase in current densities required during operation. On the contrary, recent observation by Chen (10) as well as Leong (11) that contact resistance of bonded Cu interface can decrease significantly under current stressing, suggests another method for post thermocompression bond enhancement. The subsequent section will derive a mathematical model for contact resistance reduction under direct current stressing.

**Derivation for Single Contact**

Microstructurally, a contacting asperity can be approached as a circular body with summit radius curvature of $R$, contact radius of $a$ and neck radius of $u$, that is under current stressing. The contact area of the asperity could grow by diffusion of atoms from the body to the neck region of the asperity as illustrated in Figure 3.
Figure 3. Contacting asperity diagram under current stressing. (a) Asperity cross section where electron flow is indicated by the thick arrow, (b) small finite element on the asperity surface.

The general electromigration’s atomic flux due to the electron wind force on the interconnect line is given by (22)

$$ J = -\frac{DC}{kT} Z^* eE $$

[6]

where $D$ is the diffusivity, $C$ is the atomic density, $k$ is the Boltzmann’s constant, $T$ is the temperature, $Z^*$ is the effective charge, $e$ is the electron charge and $E$ is the electric field. Considering only surface diffusion that matters, $C$ in equation [6] can be substituted by surface density $\nu$ (conveniently $\nu \equiv \Omega^{-2/3}$) (23). For simplicity, $D$ and $\nu$ are assumed to be isotropic parameters (24). Thus equation [6] becomes

$$ J_s = -\frac{D\nu}{kT} Z^* eE $$

[7]

Now consider a small finite element of the neck region as shown in Figure 3(b). Atomic flux due to electron wind force convergent on this element will drive the outward movement of the surface. It can be considered that an atomic flux $J_{e1}$ is crossing the edge of the element at the width $\delta_1$ at radial distance $r_1$ and flux $J_{e2}$ is crossing the edge $\delta_2$ at radial distance $r_2$ from the center of symmetry. By conservations of volume, it can be obtained that

$$ (J_{e1} \delta_1 - J_{e2} \delta_2) \delta t \cdot \delta V = \delta \Omega \cdot \delta n \cdot \delta l $$

[8]
where $\mathbf{\delta}$ is the average chord length of the element, $\mathbf{n}$ is the outward normal distance traveled by the element during the time increment $\mathbf{\delta t}$, and $\mathbf{s}$ is the incremental arch length measured along a section through the axis of revolution ($z$-axis). Since both $\mathbf{\delta}_1$ and $\mathbf{\delta}_2$ can be considered to subtend the same angle, we can rewrite equation [8] as

$$
(J_1 r_1 - J_2 r_2) \mathbf{\delta} \cdot \mathbf{\Omega} \cdot \mathbf{\delta} = \mathbf{\delta} \cdot \mathbf{n} \cdot \mathbf{\delta} \mathbf{n}
$$

Utilizing the relation $\mathbf{\delta} = \mathbf{\delta}_1/r_1 = \mathbf{\delta}_2/r_2 = \mathbf{\delta}/\mathbf{r}$ and re-arranging equation [9], the rate of outward surface normal movement of the small finite element can be expressed as

$$
\frac{\mathbf{\delta} \mathbf{n}}{\mathbf{\delta} \mathbf{t}} = - \frac{\mathbf{\Omega}}{\mathbf{r}} \frac{\mathbf{\delta}(J, r)}{\mathbf{\delta} \mathbf{s}}
$$

For infinitesimal body, it can be assumed that $\mathbf{\delta} = \mathbf{\delta_t}$. Thus, substituting equation [7] into equation [10] and passing the infinitesimal changes, it can be obtained that

$$
\frac{\partial \mathbf{n}}{\partial t} = \frac{\mathbf{\Omega}}{\mathbf{r}} \frac{\partial}{\partial z} \left( \frac{D \nu}{k T} Z^* e E \right)
$$

The outward movement of surface element has the same direction as the change in the contact radius $a$, thus it is safe to assume that $\partial \mathbf{n}/\partial t = \partial a/\partial t$. Furthermore, a few terms on the right hand side of equation [11] are independent of $z$, i.e. $D$ and $\nu$ are assumed to be isotropic. Note that, due to the rotational symmetry about $z$-axis, only $E$ is dependent on $z$. On the other hand, $E$ can also be expressed as $E = \rho j$, where $\rho$ is the material’s resistivity and $j$ is the electrical current density. Thus equation [11] becomes

$$
\frac{\partial \mathbf{n}}{\partial t} = \frac{\partial a}{\partial t} = \frac{D \Omega V Z^* e \rho}{k T} \frac{\partial j}{\partial z}
$$

Considering the rotational symmetry about $z$-axis and also the hemispherical approximation of asperity tips, $j$ can be expressed as

$$
j = \frac{-I}{\pi (R \sin \theta)^2}
$$
where \( I \) is the current flowing through a single contacting asperity, and \( \theta \) is the angle between \( R \) and the vertical axis as defined in Figure 3(a). A negative sign is used to indicate that the direction of electron flux is considered instead of the traditional current direction. Substituting equation [13] into equation [12], applying the trigonometric relation of \( z = R \cos \theta, dz = -R \sin \theta \, d\theta \), \( a = R \sin \theta, \partial a = R \cos \theta \partial \theta \) and rearranging for similar terms, it can be obtained that

\[
\sin^4 \theta \partial \theta = -BI \partial t, \tag{14}
\]

where \( B = 2\Omega vDZ^* \rho e/\pi kTR^4 \). Integrating both sides of equation [14] and assuming that \( a << R \) such that \( \sin \theta = \tan \theta = a/R \), \( \cos \theta = 1 \) thus

\[
-\frac{a^3}{4R^3} = -Blt + C, \tag{15}
\]

where \( C \) is the integration constant which can be determined by initial condition from equation [2] that \( a = a_0 = \sqrt{2R(z - d)} \) when \( t = 0 \). Substituting equation [15] with the initial condition and rearranging for \( a \), it can be obtained the evolution of contact radius as

\[
a(t) = \left( a_0^3 + \frac{8\Omega vDZ^* e\rho l}{kT\pi R} t \right)^{1/3}, \tag{16}
\]

which basically gives the asperity contact’s radius evolution under direct current stressing. Given the asperity tip curvature radius, the evolution of true contact area and the contact resistance can be calculated based on equation [4].

Equation [16] can be easily generalized for the case of current ramping. Assuming linear current increment is applied to the contacting asperity, that is the current can be expressed as \( I = ct \), where \( c \) is the current increment rate and the right hand side integration of equation [15] can be modified into \(-Bct^2/2\). Thus for the case of current ramp, equation [16] becomes

\[
a(t) = \left( a_0^3 + \frac{4\Omega vDZ^* e\rho c}{kT\pi R} t^2 \right)^{1/3}, \tag{17}
\]

**Derivation for Multiple Contacts**
In the case of multiple contacts, the supplied external current is split among the contacting asperities. Kirchoff’s current law (25) requires that the total current passing through the contact is the summation of current that passes through each asperity, and can be expressed as

$$I_{\text{tot}} = \sum_{i=1}^{N_i} I_i,$$  \[18\]

where $I_i$ represents the current on each contacting asperity and $N_i$ is the number of contacting asperity as defined in equation [1]. It can be assumed that the current density is uniform throughout the true contact area and that the current density $j$ can be expressed as $j = I_{\text{tot}} / A_c = I_{\text{tot}} / \sum_{i=1}^{N_i} \pi a_i^2$, where $A_c$ is the true contact area. This assumption is reasonable as smaller contacts will have higher resistances which led to the smaller currents. On the other hand, bigger contacts will have lower resistances which led to higher currents. Thus, the current that passes through each contacting asperity can be given as

$$I_i = \frac{I_{\text{tot}}}{N_i} \frac{\pi a_i^2}{\sum_{i=1}^{N_i} \pi a_i^2} = \frac{I_{\text{tot}} a_i^2}{\sum_{i=1}^{N_i} a_i^2},$$ \[19\]

As a result, the contact radius of each contacting asperity under current bias and linearly increasing current in the multi-spot contact can be expressed as shown in equations [20] and [21] respectively.

$$a_i(t) = \left( a_0^3 + \frac{8 \Omega v D Z' e \rho \tau}{k T \pi R} \frac{I_{\text{tot}} a_i^2}{\sum_{i=1}^{N_i} a_i^2} \right)^{\frac{1}{3}},$$ \[20\]

$$a_i(t) = \left( a_0^3 + \frac{4 \Omega v D Z' e \rho \tau}{k T \pi R} \frac{c_{\text{tot}} a_i^2}{\sum_{i=1}^{N_i} a_i^2} \right)^{\frac{1}{3}},$$ \[21\]

The total contact resistance can be calculated by substituting the appropriate term for $a$ into equation [5].
Simulation

A simulation on the true contact area growth due to electromigration was carried out by assuming a surface roughness of 2 nm-rms with $\sigma = 2$ nm, $\eta = 10$ m$^{-12}$ and $R = 50$ nm. The simulation was carried out with an increment current stressing of 0.1 A/s on a $100 \times 100$ $\mu$m$^2$ nominal contact area. The initial contact resistance was predetermined from the value of $d$. Generally, a smaller $d$ corresponds to lower initial contact resistance as if achieved by a combination of larger bonding force, longer bonding duration or higher bonding temperature. All of the diffusion data used in the simulation were extracted from various sources and summarized in Table I.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value for Cu</th>
<th>Units</th>
<th>References</th>
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<tr>
<td>Atomic volume</td>
<td>$\Omega$</td>
<td>$1.18 \times 10^{-2}$</td>
<td>nm$^3$</td>
<td>(26)</td>
</tr>
<tr>
<td>Diffusion</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pre-exponential</td>
<td>$D_o$</td>
<td>$10^7$</td>
<td>m$^2$s$^{-1}$</td>
<td>(27)</td>
</tr>
<tr>
<td>Activation energy</td>
<td>$E_A$</td>
<td>0.58</td>
<td>eV</td>
<td>(27)</td>
</tr>
<tr>
<td>Resistivity</td>
<td>$\rho$</td>
<td>$1.7 \times 10^{-8}$</td>
<td>$\Omega$m</td>
<td>(28)</td>
</tr>
<tr>
<td>Electron mean free path</td>
<td>$l$</td>
<td>38.7</td>
<td>nm</td>
<td>(28)</td>
</tr>
<tr>
<td>Effective charge</td>
<td>$Z^*$</td>
<td>1</td>
<td></td>
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</tr>
</tbody>
</table>

Simulations on the model show that the resistance drop is dependent on the initial contact resistance. Contact resistance starts to decrease significantly when it reaches a certain critical current as shown in Figure 4(a). The critical current has an inverse trend with the initial resistance value as observed in (11). In this case, the critical current decreases as the initial resistance increases. Beyond the critical current, the exponential decrease in resistance is consistent with the observation reported in (29). Effect of contact resistance changes with contacts temperature was also investigated.

Figure 4. Simulation result of contact resistance reduction model as a result of current stressing (a) effect of initial contact resistance, (b) incorporating contact heating effect, no significant changes of contact resistance observed. Contact resistance changes still dominated by electromigration effect.
Changes in contact resistance with changes in contact temperature can be expressed as (11).

\[ R_c = R_{c0}(1 + \alpha \Delta T) \quad [22] \]

where \( R_c \) is the contact resistance, \( R_{c0} \) is the initial contact resistance, \( \Delta T \) is the temperature changes of the contact and \( \alpha \) is the temperature-resistance coefficient. Leong (11) had roughly estimated the value of \( \alpha = 0.00411 \, \Omega/K \). Temperature changes of the contact can be estimated as the difference between the contact’s absolute temperature \( T_M \) and temperature far from the interface \( T_0 \). Whereby, from classical contact theory (12), absolute temperature of the contact is given by \( T_M = \left( T_0^2 + V_c^2 / 4L_0 \right)^{1/2} \), where \( L_0 = 2.45 \times 10^{-8} \, V^2/K \) is the Lorenz constant (12). By setting the voltage drop in the contact \( V_c = R_{c0}I \), where \( I = ct \) and \( \Delta T = T_M - T_0 \), thus equation [22] becomes

\[ R_c = R_{c0}\left(1 + \alpha\left[ T_0^2 + (R_{c0}I) / 4L_0 \right]^{1/2} - T_0 \right) \quad [23] \]

Figure 4(b) shows the simulation results incorporating contact’s heating effect to changes in contact’s resistance. It shows no significant changes of contact resistance. Contact resistance change is still dominated by electromigration mechanism.

**Model and Experiment Comparison**

Chen *et. al* (10) reported that the contact resistance reduction happens on the bonding structure that has a surface roughness of 1.15 nm - rms. Surface roughness parameters such as asperity tip curvature radius \( R \), asperity density \( \eta \) and the asperity height distribution \( \sigma \) were taken from Leong statistical data (29) for the same rms-roughness.

Figure 5 shows the model prediction and measured contact resistances of bonded interconnects extracted from (10) when the stress current was ramped gradually from 1 to 100 mA at a rate of 1 mA/s. It was observed that the contact resistance decreases and converges to a constant value at high stress current, which are well described by the model. The model was found to fit well with a pre-exponential diffusivity of \( D_o = 85 \, m/s \), giving a room temperature (27 °C) diffusivity of \( 1.58 \times 10^{-8} \, m^2/s \) and activation energy \( E_a = 0.58 \, eV \). This pre exponential factor is five orders lower than what was reported in (30). This difference is mainly attributed to the difference in driving force for surface diffusion i.e. surface curvature in (30) versus electron wind force in the current model. Nevertheless, the current model has justified theoretically the electromigration-induced reduction in the initial contact resistance of bonded interconnects. The model also provides a mechanism for post-bonding bond property improvement for 3D-ICs.
Summary and Conclusion

Cu thermocompression bonding is seen as a general route to realize 3DIC as bonded metals provide both mechanical adhesion and electrical interconnection. Contact resistance reduction by current stressing opens up a new method for post-bonding Cu bond interface enhancement. Electromigration assisted contact resistance reduction based on the phenomenon observed in (10, 11, 29) has been modeled. The model describes well the experimental observation of an exponential resistance decrease when it reaches a certain critical current density. The critical current dependence on the initial resistance value is also well captured by the model. Besides providing the theoretical justification of the electromigration-induced reduction in the initial contact resistance of bonded interconnects, the model also provides a mechanism for post-bonding bond property improvement for 3D-ICs, as well as prediction tools for production.

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