An Investigation on Nanoscale Tensile Mechanical Properties for Pd-coated Copper Wire

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Abstract

The mechanism of intermetallic compound (IMC) between Copper (Cu) free air ball (FAB) and Aluminum (Al) bond pad has been carefully investigated in this paper. The test vehicle is Pd-coated Cu wirebonds on Al pad in plastic ball grid array (PBGA) package. Palladium (Pd), the anti-oxide material coated on Cu wire will be blended in the Cu FAB when the ball is formed by an electrical flame-off (EFO). Preliminary results demonstrated that Cu-Al IMC cracks originally begins from the edge of bonding interface and spreads into the center area. This is the cause of open fail. Nanoscale bondabilities on IMC of Cu/Cu₉Al₄ and CuAl₂/Al are also cautiously investigated by using molecular dynamics (MD) simulations. Nanoscale tensile force and tensile strength are predicted to examine the bonding strength of two IMCs along the bonding interface. Interfacial fracture is different in different tensile speed as well as the working temperature. A series of experimental works and MD simulations are conducted in this research.

Introduction

Wirebonding process using ultra-thin copper wire has been implemented in semiconductor packaging industry for the past few years for its easy application and low cost. However, higher rigidity and strength of Cu wire would result in Al pad squeezing beneath the mashed FAB. Cu oxidization issue can be improved by coating Palladium (Pd) over the copper wire surface. However, failures caused by higher rigidity of Cu material and intermetallic compound (IMC) layer along Cu-Al interface have been caught attention by many researchers [1-3]. It is reported that the hardness of CuAl IMC is also stiffer than either copper or aluminum material. The influence of Cu-Al IMC is fully examined by OM, SEM, TEM and EDS. It is observed that the diffusion rate of Cu into Al is faster than that of Al into Cu. Preliminary results shows the thickness of IMC affect the bondibility of copper wire and the void is propagated along copper FAB boundary. As soon as FAB is formed by EFO, the Pd coatings would spread into Cu ball based on TEM-EDX analysis. Only a small portion of Pd concentration can be occasionally examined at the bonding interface. It is observed that IMC layers are spontaneously formed beneath the crushed FAB surface. A thin layer of IMC is observed in the center area. The lower IMC layer is considered as CuAl₂ protruded from Al pad surface. IMC layer in the upper side is determined as Cu₉Al₄. The atomic ratio of Cu-Al in the middle IMC layer would be varied or intermixed of the two phases of IMCs. Al splashes are easily found at the outside of Cu ball bonds. Thus, crack begins from the edge and gradually propagates inside along the line of IMC bonding interface. Voids are observed at all interfaces between Cu and Cu-Al alloy phase. Therefore, the bonding strengths of Cu/Cu₉Al₄ and CuAl₂/Al have essential interests to define the bonding interface.

Because many material properties of Cu wire and Al pad are scarcely realized, wirebonding process is essentially difficult to simulate by numerical approach. As the characteristic size of the thin film reduces to nanoscale, finite element method is not capable to investigate the strain-stress behavior on the nanostructure. Molecular dynamics (MD) has been widely applied to simulate the material behaviors in a variety of materials in nanoscale movement [4]. Temperature and tensile speed are two major factors on determining the bonding strength. Material in high temperature has greater kinetic energy and has better formability. Higher pulling speed in tensile test would results in material much easier fracture. Based on density functional theory in quantum mechanics, potential function is derived to describe metallic properties and behaviors.
Experimental works

For comparison, ultra thin ($\psi = 15\mu m$) 99.99% (4N) Pd-coated Cu wire and 4N no-coating Cu wire were selected for the test materials. Electric flame off (EFO) processes for Cu wires were conducted by K&S 1488 plus wire bonder.

Micro-tensile mechanical property

Build up layers are laminated on core consisting of several conductive layers with a vacuum hot press. Based on ASTM standard F219-96, microscale tensile pull tests were conducted for Cu wires. Samples were prepared in 10mm length, wire pull speed is controlled in 1mm/min and the yield strength is measured at 1% of total elongation. All data were repeatedly measured at least three times to receive consistent results. The Instron-3365 universal test system with 5N±0.5% load cell is used. Thermal effects (25, 150, 175 and 200°C) on material properties are taken into account. The chamber needs to be Nitrogened to avoid oxidization.

Figure 1 shows the true stress-true strain curve of micro-tensile pull tests for Pd-coated/no-coating Cu wire at 25°C. The corresponding micro tensile mechanical properties for all cases studies are listed in Table 1.

<table>
<thead>
<tr>
<th>Cu Wire</th>
<th>T(°C)</th>
<th>E(GPa)</th>
<th>Yield Strength (MPa)</th>
<th>0.2% Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>no-coating</td>
<td>25</td>
<td>75.76</td>
<td>215.70</td>
<td>121.33</td>
</tr>
<tr>
<td></td>
<td>150</td>
<td>65.67</td>
<td>174.37</td>
<td>102.32</td>
</tr>
<tr>
<td></td>
<td>175</td>
<td>56.51</td>
<td>168.14</td>
<td>100.75</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>52.12</td>
<td>157.54</td>
<td>97.98</td>
</tr>
<tr>
<td>Pd-coated</td>
<td>25</td>
<td>80.85</td>
<td>245.88</td>
<td>162.54</td>
</tr>
<tr>
<td></td>
<td>150</td>
<td>66.32</td>
<td>196.35</td>
<td>144.26</td>
</tr>
<tr>
<td></td>
<td>175</td>
<td>64.32</td>
<td>189.06</td>
<td>140.92</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>54.91</td>
<td>173.68</td>
<td>139.93</td>
</tr>
</tbody>
</table>

Theoretical derivation

Among many potential models in MD simulations, Tight-Binding (TB) model derived by Rosato [5] is used in this research to investigate the dynamical properties, surface energies and reaction forces behavior of face-centered cubic (FCC) atoms by many-body potential energy functions. For metal material, TB model is capable to explore the variation of mechanical properties during tensile test. The potential energy, attractive energy, repulsive energy and atom-scale stress are expressed as follows

\[ E_c = \sum_i (E_R^i + E_B^i) \]  
\[ E_R^i = \sum_{j \neq i} U_{ij}(r_{ij}) \]
\[ U_{ij}(r_{ij}) = Ae^{-\left(\frac{r_{ij}}{r_0} - 1\right)} \]

\[ E_R^i = \sum_{j}^{} \left( \frac{\phi_{ij}(r_{ij})}{2} \right)^{1/2} \]
\[ \phi_{ij}(r_{ij}) = \xi^2 e^{-2q\left(\frac{r_{ij}}{r_0} - 1\right)} \]

Substitute equation (2) and (3) into (1) receives full tight-binding potential in equation (4).
where $A$, $p$, $q$, $\xi$, $r_0$ are experimental constants, or obtained from fitting using tight-binding potentials.

**Molecular dynamics**

MD has been widely applied to evaluate the material behaviors in a variety of materials in atomic-level motion. Temperature and tensile speed are two major factors on determining the bonding strength between two materials. Material in high temperature possesses a greater kinetic energy and holds a better formability. Higher pulling speed in tensile test would result in material easier fracture. Based on density functional theory in quantum mechanics, potential function is derived to describe metallic properties and behaviors. Figure 2 illustrates the predicted tensile model using MD simulation for pure Al, Cu-Al (IMC) and pure Cu materials. The thickness of IMC Cu-Al layer is less than 8Å. Figure 3 demonstrates the boundary conditions and number of atoms used in the predicted tensile model. Both Cu and Al atomic scale used in this study is real size. Experimental constants (bonding properties) $A$, $p$, $q$, $\xi$, $r_0$ in equation (4) are listed in Table 2 for Cu, Al and Cu-Al [6].

![Figure 2 Real size of the predicted tensile MD model.](image)

![Figure 3 Boundary conditions and number of atoms used in the predicted tensile MD model.](image)

### Table 2 Bonding properties in tight-binding potential function.

<table>
<thead>
<tr>
<th></th>
<th>Cu</th>
<th>Al</th>
<th>CuAl</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ (eV)</td>
<td>0.0783</td>
<td>0.160199</td>
<td>0.525141</td>
</tr>
<tr>
<td>$P$</td>
<td>11.183206</td>
<td>7.568105</td>
<td>6.178625</td>
</tr>
<tr>
<td>$\xi$ (eV)</td>
<td>1.2355</td>
<td>1.5074</td>
<td>1.43527</td>
</tr>
<tr>
<td>$Q$</td>
<td>2.319698</td>
<td>2.7456</td>
<td>1.60164</td>
</tr>
<tr>
<td>$r_0$ (Å)</td>
<td>2.556</td>
<td>2.8634</td>
<td>2.14769</td>
</tr>
</tbody>
</table>

The presented bonding property of Cu-Al IMC is fitting by using the existing potential [7].

**Atomic-level strain/stress**

Based on theory of Continuum Mechanics, the entire material is assumed to be continuous without any defect (void) in macro view. However, the strength of material is not capable to describe the strain/stress behavior in nanoscale of molecular/atomic motions. Figure 4 illustrates the predicted atomic-level enlarged length (including length and elongation) from $n$ step to $n+1$ step. Atomic-level strain calculation can be then easily obtained from equation (5).

Atomic-level stress calculation in this research is BDT stress model derived by Miyazaki [8]. The idea of BDT stress model is a single atomic stress can be obtained to accumulate the average stress in the localized area. Figure 5 demonstrates the accumulated average stress in localize area $S$ for a single atom. The atomic level stress in the localized area can be obtained from equation (6).
Figure 4 Atomic-level length from n step to n+1 step.

\[ \epsilon_{(n+1)} = \frac{(l_{n+1} - l_n)}{l_n} \]  

(5)

Figure 5 Accumulated average stress in localize area S for a single atom. From a single atom, the average atomic-level stress in the localized area is

\[ \sigma_{mn} = \frac{1}{N_S} \sum_i \left[ \frac{M_i v_i^m v_i^n}{V_i} \right] \left[ \frac{1}{2} \sum_j \frac{\partial \phi(r_{ij})}{\partial r_{ij}} x_{ij}^m x_{ij}^n \right] \]  

(6)

where \( N_S \) is the number of atoms in region S, \( M_i \) is the atomic weight of atom i, \( v_i^m \) is the velocity in m direction for atom i, \( r_{ij} \) is the relative distance between atoms i and j, \( \phi(r_{ij}) \) is the potential and \( x_{ij}^m \) is the displacement in is m direction for \( r_{ij} \). \( V_i \) is the total atom volume in the stressed region and \( a_i \) is the average radius of atom in stressed region.

\[ V_i = \frac{4\pi}{3} a_i^3 \]

Material properties of different contents of Cu-Al IMC were listed in Table 3 [6]. As can be seen, the hardness of IMC is larger than that of pure materials, for instance, microhardness of CuAl is 628 HV5. The hardness of Cu is 60-100 HV5 and the hardness of Al is 20-50 HV5. The IMC is much harder than pure Cu and pure Al materials. In MD simulation, the crystal structure of CuAl is monoklinic which is different from BCC of pure Cu and Al.

<table>
<thead>
<tr>
<th>Concentration (at.% Cu)</th>
<th>Crystal Structure</th>
<th>Hardness HV5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>0.0 - 2.84</td>
<td>Cubic</td>
</tr>
<tr>
<td>CuAl_2</td>
<td>31.9 - 33.0</td>
<td>Tetragonal</td>
</tr>
<tr>
<td>CuAl</td>
<td>49.8 - 52.3</td>
<td>Monoklinic</td>
</tr>
<tr>
<td>CuAl_4</td>
<td>62.5 - 69</td>
<td>Cubic</td>
</tr>
<tr>
<td>Cu</td>
<td>80.3 - 100</td>
<td>Cubic</td>
</tr>
</tbody>
</table>

Table 3 Material properties of Cu-Al IMC.

Results and discussion

The surface between CuAl IMC is assumed to be perfectly flat without any roughness. Relaxation movement was performed to assure the stability of MD tensile test simulation. After the entire structure was reaching stable equilibrium, the atomic weight of Cu=63.546, Al=26.9811, \( v=0.00001\text{Å}/\text{fs} \) and initial temperature \( T=300\text{K} \) were applied to the model.
Figure 6 Tensile test simulations using MD. (a) relaxation (b) pull (c) necking (d) before rupture (e) after breakage (f) cease.

Figure 6 illustrates the predicted tensile test using MD simulation for pure Al, Cu-Al IMC and pure Cu. MD predicted results are also shown that pressing depth between two bonding materials will affect the bonding strength. This is very important for thermoelectric ball bond process. Figure 7 shows the predicted nanoscale elastic property.

Figure 7 Predicted nanoscale elastic property.

Summary

As the CuAl IMC emerged from bonding process, mechanical properties of Cu-Al were found to be much better than Cu and Al materials. From Figure 6 (a) to (f), necking is observed in the Al atoms and rupturing is also found in the region of Al atoms. Bonding strength of CuAl IMC is better than pure Al, but is weaker than pure Cu. MD simulations to predict the nanoscale IMC bondability in this research are demonstrated.

Acknowledgments

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References