

Study of Capillary Underfill Filler Separation in Advanced Flip Chip Packages

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Abstract — The key role that underfill materials play in highly reliable, advanced flip chip organic packages has generated an increased focus on their behavior and structure. One such behavior relates to the observation of filler separation from the resin matrix which, to date, has been predominantly attributed to gravity or capillary flow.

The phenomenon of silica filler separation is discussed in the context of fine pitch, lead-free solder joints with copper-base (pedestal or pillar) under bump metallization and large die packages. The principle mechanism driving filler separation in these structures was confirmed as a migration of the electrostatically charged filler particles away from the copper regions and towards the solder regions of the interconnect.

Based on this finding, various factors that influence the surface of the interconnects or the nature and the mobility of the filler particles during the bond and assembly process were explored. It was found that the oxide states and contact angles of the interconnect surfaces do not appear to impact the degree of filler separation. Within the range explored, average filler particle size is ineffective in changing the separation behavior. On the other hand, lower filler content somewhat increases the extent of separation and is believed to be related to an increase in particle mobility. Assembly process variables with known effects on surface interactions and underfill flow were also studied, revealing no observable shift in the occurrence of filler separation.

Finally, and most importantly, a reliability study was conducted to investigate the impact of this phenomenon in a very large die (23 x 23 mm²) flip chip organic package subjected to a high level of thermomechanical stress. Using extended Deep Thermal Cycling to 2000 cycles (as opposed to the standard 1000 cycle criterion), no packaging failures occurred and no signs of interconnect degradation were observed. These results are consistent with finite element modeling of the tested package, which showed that stress changes from filler separation in regions of similar dimensions to those that were experimentally observed were within the limits of model error and typical manufacturing variability.

Keywords- *Underfill; Filler separation; Cu pedestal, Pb-free, Large die reliability, Finite Element Modeling*

I. INTRODUCTION

After years of development, underfill encapsulant materials and their related processes remain critical enablers for high end, highly stressed advanced flip chip packages. Underfills are generally two phase composite materials. They comprise an epoxy resin main phase, which is loaded with micron and sub-micron size spherical silica particles in the order of ~60 weight %. The main role of the fillers is to optimize the mechanical properties of the encapsulant for robust packaging, generally by increasing the rigidity of the material and by lowering its thermal expansibility. Filler technology development in high end underfills is arguably the formulator's most guarded secret as it is such a determining factor in underfill processing and module reliability. Controlling the filler dispersion in the resin matrix during the material synthesis, storage and module assembly is certainly one key aspect to obtaining the full potential of the designed composite. Yet it is not infrequent to observe some level of filler separation, i.e. a migration from its homogeneously dispersed state, to which various causes have been attributed, such as gravity (filler settling), capillary flow and particle surface mechanisms.

Previous work addressing the impact of such separation on underfill properties and performance, predominantly through FEM (Finite Element Modeling), reports local changes in mechanical properties, but the correlation to reliability is not clear, as the effect of separation is often obscured by other factors. For instance, Schubert et al. [1] predict that the lower elastic modulus and higher CTE of the resin-rich zone will promote not only larger joint creep strains that can lead to solder cracking, but also induce a higher tensile peel stress that might cause underfill delamination. However, the reliability impact is only indirectly implied by proposing that increased filler content did not improve reliability due to its increased amount of filler settling. Chen et al. [2] similarly report higher peel stresses in modeled underfills with filler settling, but suggest that the effect can be offset by the underfill fillet. These authors also predict reduced cycling performance for bi-layered settling models with an abrupt change in filler content at the layer boundary, but not for gradual filler settling. That said, they further report that a higher Young's modulus of the underfill can mitigate said performance

impact. Another study [3] demonstrated that the reliability impacts of filler separation are mitigated by a suitable particle size distribution, such as practiced by many underfill suppliers today, instead of a single particle size.

The previously cited work has focussed on packages with eutectic lead-based solder interconnections and filler separation was addressed as a vertical settling mechanism. The advent of finer (50-150 μ m) interconnect pitch packages with increased current density has forced the introduction of novel Cu-base under bump structures (Cu pedestals, Cu pillars). These new structures have been associated with new filler surface separation mechanisms, as reported by Namics [4]. The difference in standard electrode potential between Cu and Sn induces an electrophoretic effect that causes the electrostatically charged filler particles to migrate away from Cu regions and towards the solder regions of these new interconnects. It is hypothesized as part of this study that such an effect might be exacerbated by the higher Sn content in Pb-free solder interconnects. An example of filler separation for a Cu pedestal/Pb-free interconnect is illustrated in Fig. 1. While finite element modeling in reference [4] suggests increased stress in specific locations in the presence of such separation, no reliability evaluations were reported.

This study therefore focusses on this new filler separation mechanism as it applies to Pb-free interconnects with thick Cu UBM (Under Bump Metallization) in large die packages. Our goals are to (1) further understand and explain the phenomenon and its influencing factors and (2) determine whether such separation has a reliability impact in actual stress testing. Additionally, we propose an FEM model specific to the nature of the separation and compare its predictions to the stress performance results.

II. EXPERIMENTAL METHODOLOGY

Two test vehicles were selected to investigate the filler separation mechanism in the presence of thick Cu UBM from the perspective of high end package manufacturability and reliability.

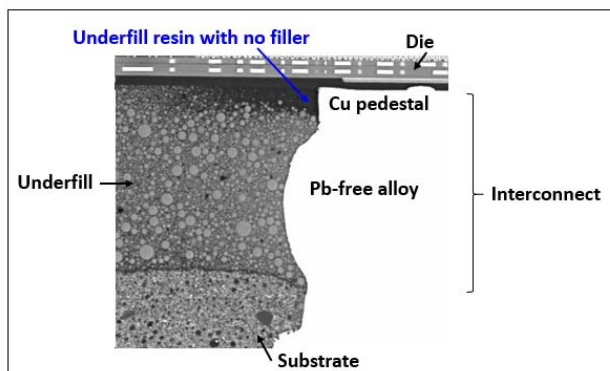


Figure 1. Underfill filler separation from the resin matrix near the Cu region of the interconnect.

A first test vehicle (TVA) of modest dimensions was used to investigate the electrophoretic effect, while a second one (TVB), with a large 14 nm BEOL (Back End Of Line) die attached to a 55 x 55 mm² organic substrate, was selected to explore the most challenging manufacturing and reliability conditions. Importantly, the interconnections of both test vehicles comprised a Cu pedestal (base) portion and a SnAg solder portion. The specific characteristics of TVA and TVB are detailed in Table 1.

Modules were assembled with appropriate bond and assembly processes and materials for large die packages. A package schematic and the process flow are shown in Fig. 2.

TABLE 1. TVA AND TVB TEST VEHICLE DESIGNS

Test Vehicle	TVA	TVB
Chip size (mm x mm)	9 x 14	23 x 23
Interconnect metallurgy	Cu pedestal SnAg solder	Cu pedestal SnAg solder
Interconnect pitch (μ m)	150	150
Substrate size (mm x mm)	31 x 31	55 x 55
Substrate cross section	4-2-4	4-2-4
Substrate core thick. (μ m)	800	400
Lid size (mm x mm)	-	53 x 53
Lid thickness (mm)	-	1

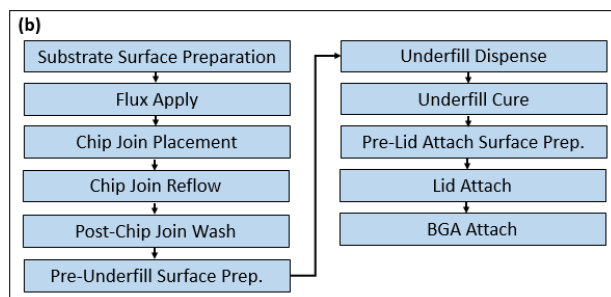
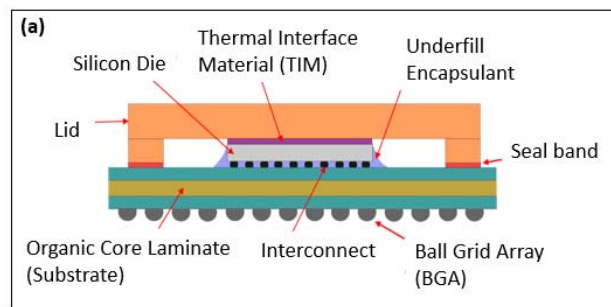


Figure 2. TVA assembly showing (a) schematic of module construction and (b) process flow.

Module cross sectioning after underfill cure was used to assess filler separation for the different experiments since fillers are no longer mobile in the resin matrix at this stage. While a number of inspection techniques were evaluated to characterize the separation, SEM (Scanning Electron Microscopy) was found to provide superior results over bright field or dark field light microscopy, as illustrated in Fig. 3.

A. Filler separation phenomenon and mechanism confirmation

A first set of experiments was designed to validate whether the main mechanism underlying the separation was indeed the electrophoretic effect on the electrostatically charged filler particles caused by the Cu in the package. Inspired by previous work [5], underfill flow/cure experiments were conducted with applied voltage on two versions of TVA: the previously described TVA test vehicle with Cu pedestal interconnects, as well as TVA assemblies where Cu lines were exposed from the laminate top build-up layers by selectively removing portions of the overlying soldermask material with a laser ablation process. In this latter case, the presence of filler separation at the bottom of the underfill layer and adjacent to the exposed Cu would eliminate gravity as a possible separation mechanism.

B. Influence of interconnect surface modification on filler separation

A second group of tests attempted to treat the surface of the TVA interconnects in order to modify their surface charge state and therefore their electrostatic interaction with the filler particles. Two approaches were studied. A first technique exposed the interconnects to an oxygen plasma treatment in an attempt to create an oxide surface on the copper and on the solder. In order to maximize the extent of oxidation, oxygen plasma was processed directly on the interconnects, without joining the die to an organic substrate. Underfill was also dispensed directly on the interconnects. The second approach applied silane based adhesion promoters to coat the interconnects.

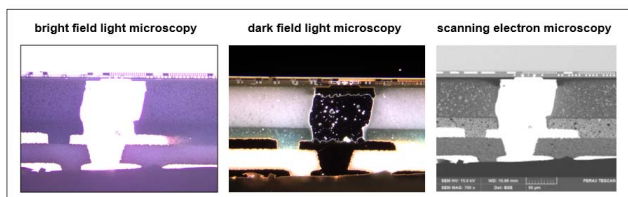


Figure 3. Underfill filler separation characterization with a) bright field light microscopy b) dark field light microscopy and c) scanning electron microscopy.

C. Influence of underfill material composition on filler separation

The third block of tests investigated the effects of underfill material composition on the electrophoretic effect for TVA modules. Table 2 describes the difference between four underfill materials that were identical with the exception of filler size (average filler size in μm) and filler ratio (in weight percent). This was premised on the hypothesis that an increased mobility of either finer particles or a less dense composite would increase the resulting level of filler separation. The rheological behavior of the four formulations at 100°C was studied using an ARES rheometer from TA Instruments. The rheometer was used in a parallel plate configuration (diameter: 50 mm; gap: 1 mm). Steady state flow tests were carried out to evaluate the viscosities in the shear rate range of 0.1 s^{-1} to 10 s^{-1} .

D. Influence of assembly parameters on filler separation

The fourth block of experiments focussed on the impact of specific assembly process parameters on the dimension and location of the filler separation regions adjacent to the Cu pedestal. The assembly process parameters that were targeted were those that could influence the underfill capillary flow during the first few seconds of the process when underfill material viscosity is at its minimum and filler mobility is (presumably) maximal. To this end, different chip join flux materials and different post chip join flux cleaning processes were evaluated, as well as different underfill process dispense patterns on TVB modules.

E. Reliability evaluation

In a final set of experiments, TVB modules were assembled under appropriate manufacturing controls and subjected to JEDEC L3 / 245C preconditioning, followed by 2000 cycles of -55 to 125°C DTC (Deep Thermal Cycling) [6]. Electrical testing and verification was performed after JEDEC preconditioning and at each 250 cycle readout. Visual inspection, scanning acoustic microscopy and cross-sections were performed after JEDEC preconditioning and at each 500 cycle readout to check for any packaging related defect.

TABLE 2. UNDERFILLS WITH DIFFERENT FILLER SYSTEMS

Underfill	Average filler particle size (μm)	Filler content (weight %)
A	2	65
B	1	60
C	1	55
D	1	45

Two modules were characterized by cross-sectional analysis at the end of DTC stress in order to assess the level of filler separation near the bump pedestal. While well beyond the typical qualification target of 1000 cycles, this stress extension to 2000 cycles was chosen in order to magnify the possible effect of the presence of filler separation on reliability.

F. Finite Element Modeling

The FEM model study used the PACK software [7], a high performance numerical software which wraps advanced pre- and post-processing capabilities around different finite element software systems (including ANSYS [8], in this work). It is used as a virtual qualification platform for microelectronic components by the IBM Corporation. Fig. 4 shows details of the mesh used for TVB. A 65µm underfill thickness with 1.5 mm long fillets were assumed. Other geometrical dimensions are as outlined in Table 1. Standard material properties for the Cu lid and silicon die were used. Material properties for the seal band and thermal interface materials were obtained from the suppliers or dedicated characterization experiments, and are not presented here (IBM proprietary information). Advanced modeling features of the PACK software were used [7]. These include over-compression non-linearities in the thermal interface layer between the die and the lid of the module. The copper distribution of each substrate build-up layer was obtained from the board files and superposed on the mesh in order to calculate the equivalent material properties of each element in the substrate. A custom mesher was used to handle the specific geometries encountered in microelectronic packages.

A micro-macro model approach was used to model an interconnect located 0.5 mm diagonally from the corner of the die, where thermo-mechanical constraints are the largest. The micro-model was coupled to the macro-model to refine stress estimates in the interconnect (it did not affect stress calculations at the macro-model level).

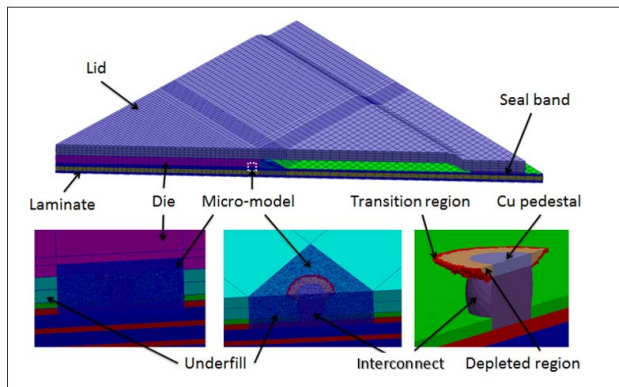


Figure 4. FEM model and zoom in micro-model.

The micro-model was composed of a portion of the silicon die, the interconnect (Cu UBM and solder joint), a portion of the underfill and a portion of the substrate (Fig. 4). The underfill filler separation was modeled by first defining three distinct regions in the underfill for the micro-model, based on geometries observed in actual cross-sections. A standard underfill region had elements with the composite (resin/filler) material properties shown in Table 3. A depleted region with a hollow truncated conical shape is in contact with the copper pedestal. Elements that are completely inside the depleted regions have material properties corresponding to pure epoxy resin (no fillers). Finally, a transition region between the depleted region and the underfill region comprised elements with at least one node in the depleted region. These elements had material properties that were linearly interpolated between those of the depleted regions and those of the underfill regions, based on the fraction of the volume of the element inside the depleted region.

III. RESULTS AND DISCUSSION

A. Filler separation phenomenon and mechanism confirmation results

The application of +5V on specific interconnects during the underfill dispense and the underfill cure of TVA modules clearly impacted the level of filler particle separation from the Cu pedestal and in some cases from the entire interconnect, as illustrated in Fig. 5. Charged filler particles were attracted by the positively biased interconnects.

The amplification of the filler separation phenomenon with the applied voltages suggests an electrostatic mechanism rather than gravity as the main cause, supporting the electrophoretic effect hypothesis. This is further demonstrated by the experiment in which Cu was exposed at the bottom of the underfill gap. Fig. 6 shows that filler particles had a lower density in the gap area over the exposed Cu lines when compared to areas with no exposed Cu. In fact, the underfill material at the bottom most region in contact with the exposed Cu line contained no filler particles whatsoever.

TABLE 3. UNDERFILL MATERIAL PROPERTIES

Underfill	Young's Modulus (MPa)	Poisson coefficient	Thermal expansion coefficient (ppm/C)
Underfill resin (no fillers)	100	0.35	64
Underfill with 65 weight % fillers	9530	0.3	29

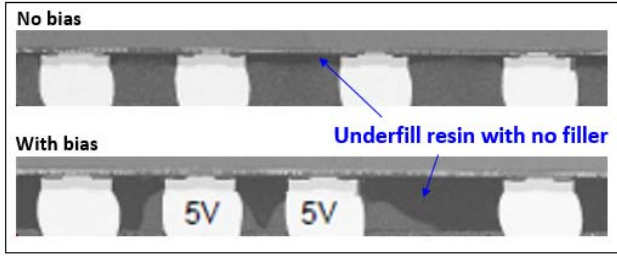


Figure 5. Increased level of filler particle separation with applied voltage (5V) on TVA modules.

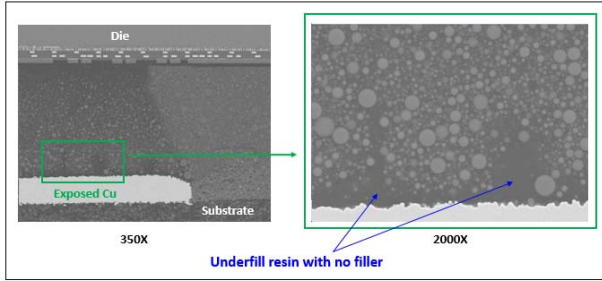


Figure 6. Filler separation in presence of Cu at the bottom of the underfill gap.

B. Influence of interconnect surface modification on filler separation results

In the case of the oxygen plasma treatment, resultant TVA cross-sections did not reveal any significant changes in the filler separation at the Cu pedestal.

For the silane based adhesion promotor experiments, water contact angle measurements were first used to assess the extent to which various treatments modified the Cu and solder surfaces (Table 4). Despite evidence of important modifications in contact angle, no significant changes in filler separation were observed. These experiments suggest that oxidation or coating of the interconnect surfaces do not alter the resultant electrical field near the interconnect regions, and therefore have no effect on the electrophoretic mobility of the filler particles. While these preliminary studies were inconclusive, additional work is recommended to more thoroughly investigate and understand the relationship between interconnect surface and filler particle electrophoretic behavior.

TABLE 4. CONTACT ANGLE MEASUREMENT WITH DI WATER

Silane based Adhesion Promotor (AP)	Cu	Sn
None (control)	0	39
AP_1	69	63
AP_2	87	73
AP_3	91	83

C. Influence of underfill material composition on filler separation results

Several TVA cross-sections and SEM observations were performed on the 4 underfill materials described in Table 2, for which representative images are shown in Fig. 7. No significant difference between underfill A and underfill B was observed, suggesting that there is no impact on the filler separation mechanism in the Cu pedestal area when average filler size is reduced by 50%, in the 1 – 2 μ m range.

On the other hand, a comparison of underfills C and D versus B reveals an increase in the level of filler separation with a reduction in the filler content. Rheological measurements, as presented in Fig. 8, demonstrate a clear trend of lower viscosity with lower particle loading. It is therefore hypothesized that a 10 to 15% reduction in particle loading could increase filler separation by means of a higher mobility of the filler particles. This may be related to the lower viscosity of the composite, but might also be caused by the inherent change in electrophoretic mobility of the charged particles. Theoretical modeling studies [9, 10] have suggested that, in concentrated colloidal suspensions at low frequency electrical fields, the dynamic electrophoretic mobility of the particles tends to increase as particle volume fraction decreases.

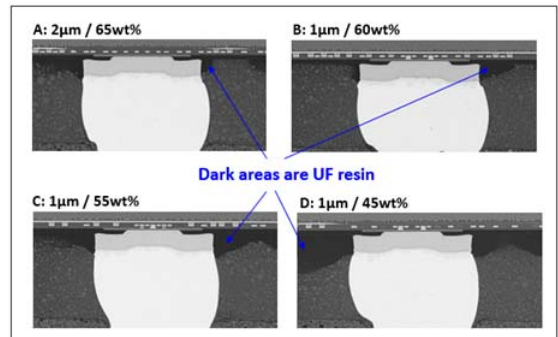


Figure 7. Filler separation with different filler sizes (average size in μ m) and filler concentration (weight %).

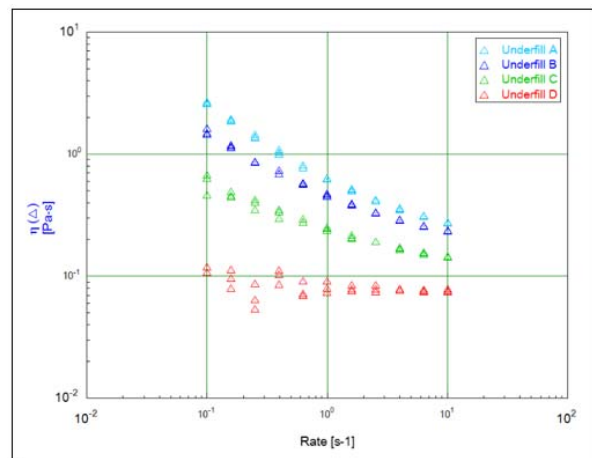


Figure 8. Rheological behavior (viscosity, η) at 100°C of underfills with different filler content.

D. Influence of assembly parameters on filler separation results

The different assembly process verifications are documented in Table 5 along with their corresponding impacts on filler particle separation. As seen in cells 1 through 4, chip joining process modifications did not appear to have any effect on the extent or location of the filler separation at the interconnect interface. Specifically, a flux with higher oxide reduction action and improved interconnect wettability (cell 2) did not modify the reference cell 1 filler separation response. A 90 degree or 180 degree deionized water flow rotation (cell 3) was equally unresponsive. Even with the exaggerated condition of cell 4, where chip joining was performed in the absence of any flux or cleaning process, no change in the filler separation phenomenon was observed. While no surface analysis was performed to confirm, it is fully expected that interconnects in this cell would be maximally affected with respect to oxidation state, thereby reinforcing the observations of section B that said state has little impact on the filler particle charging effect and resultant separation.

From an underfill perspective, while dispense pattern modifications resulting in a 90 degree or a 180 degree capillary flow rotation (cells 5 & 6) altered the appearance of macroscopic flow lines versus cell 1, microscopic examination showed no modification of the filler separation configuration in the Cu pedestal region. As an ultimate case of capillary flow impact, cell 7 was produced with the underfill material dispensed directly onto the TVA interconnects facing up, thereby representing a no flow condition. Still, the filler particle separation signature resembled the control cell 1, as seen in the SEM cross-section in Fig. 9. These results, in conjunction with those reported in section C, suggest that filler separation, while influenced by filler particle mobility induced by changes in the particle loading, is not affected by the flow dynamics of the composite material, thereby providing further evidence that the studied mechanism is predominantly an electrophoretic effect rather than gravity and filler particle settling.

E. Reliability evaluation results

Table 6 summarizes the results of the DTC evaluation on TVB with underfill A. All modules were defect free with no electrical fail, no delamination, no underfill cracking and no other package related defect up to 2000 cycles of DTC.

In light of these results, two of the modules after 2000 cycles of DTC were cross-sectioned to investigate for any defect initiation, with specific focus on die corner interconnects (highest stress location). Despite the observation of representative filler separation at the Cu pedestal, as shown in Fig. 10, no structural anomalies (interconnect cracking, underfill delamination, etc.) were observed. Considering the extended conditions of this thermal cycling, it can be strongly inferred that the filler

particle separation mechanism of the tested underfill A in the presence of Cu at the interconnect pedestal is not a reliability concern. It is proposed that other properties of this underfill, specifically high adhesion and high fracture toughness, as well as optimized surface preparation conditions in assembly, are the overriding factors in reliability performance, as further supported by the absence of field failure on multiple technology nodes using this underfill.

TABLE 5. ASSEMBLY PROCESS IMPACT ON FILLER SEPARATION

Chip joining process alternatives (with optimized underfill A capillary and cure processes)		Impact on filler separation
Cell 1 (ref.)	Water soluble flux I and with optimized cleaning process	No difference between different cells
Cell 2	Water soluble flux II (higher performance flux vs flux I) and with optimized cleaning process	
Cell 3	Water soluble flux I and with alternate deionized water flow and cleaning configurations	
Cell 4	No flux and no cleaning processes	
Underfill A process alternatives (with water soluble flux I and with optimized cleaning process)		Impact on filler separation
Cell 1 (ref.)	Optimized underfill A capillary and cure processes	No difference between different cells
Cell 5	Alternate capillary dispense orientation: 90 degree capillary flow rotation	
Cell 6	Alternate capillary dispense orientation: 180 degree capillary flow rotation	
Cell 7	No flow underfill simulation (no capillary action)	

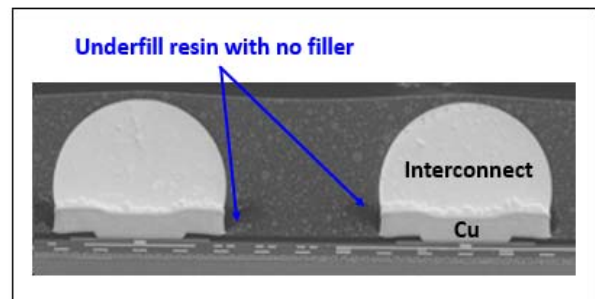


Figure 9. Underfill filler separation at the Cu pedestal with a no flow underfill process (TVA interconnects facing up).

TABLE 6. TVB STRESS EXTENSION RELIABILITY RESULTS

	T0	Jedec L3 / 245C	DTC -55 / 125C							
			250c	500c	750c	1000c	1250c	1500c	1750c	2000c
Electrical fail	0/25	0/25	0/23	0/23	0/21	0/21	0/19	0/19	0/17	0/17
Underfill delaminations	-	0/2	-	0/2	-	0/2	-	0/2	-	0/17
Underfill cracks	-	0/2	-	0/2	-	0/2	-	0/2	-	0/2
All package defects	-	0/2	-	0/2	-	0/2	-	0/2	-	0/2

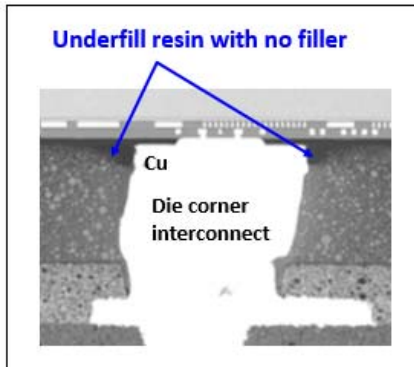


Figure 10. SEM image of a corner interconnect post 2000 cycles of DTC showing some level of filler particle separation at the top of the interconnect and no packaging related defect.

F. Finite Element Modeling results

The principal stress S1 in the underfill is shown in Fig. 11 for two models with identical meshes, where the only difference is the presence or absence of filler separation. Similar disparities were observed for the stress in the die. As previously described in section II, filler concentration is uniformly 65 weight % in the case of no filler separation, while for the filler separation case, a transition region gradually reduces filler concentration from 65% to 0% in the depleted region. Based on this model, an increase of about 12% in the principal stress is induced by filler separation. These findings are similar to those reported by Schmaltz [4] on stress increases in the low K dielectric region of the die. Nevertheless, such a magnitude of change is considered to fall within the margin of error for this and most models as well as within the range of stress variations in the manufacturing process. Moreover, if low levels of stress increases occur near the depleted region, their effects may very well be offset by an increase in underfill adhesion within that same resin-rich region, as previously measured by Nagarajan et al. [11]. In all cases, the ~10% possible increase in stress is expected to keep the stress maximum within the adhesion and fracture limits of the underfill (in line with DTC results from section E). As such, no significant concern for reliability would be anticipated by this modeling.

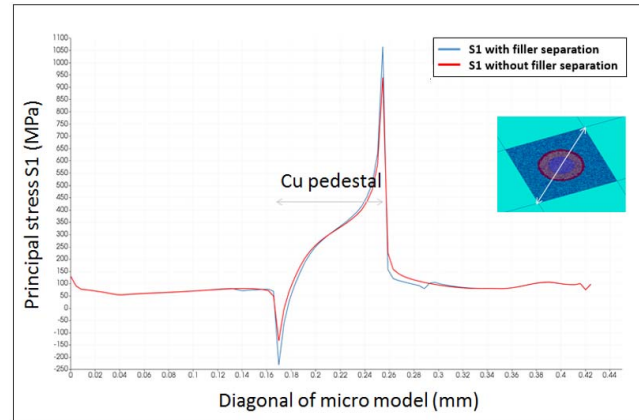


Figure 11. Principal stress S1 in the underfill and Cu UBM, along the diagonal of the micro-model.

IV. CONCLUSION

A new mechanism of underfill filler separation from its resin matrix was investigated. The electrostatic charging of the filler particles coupled with the electrode potential differences within the SnAgCu interconnections with thick Cu UBM correctly explains the filler particles migration away from the Cu pedestal region of the interconnect.

Specific testing to study this electrophoretic effect had clearly demonstrated its predominance over other well documented sources of filler separation, such as gravitational or dynamic separation caused by restricted capillary flow. A number of factors were investigated to understand their influence on this new filler separation mechanism and perhaps even lead to means of alleviating the effect. Preliminary experiments to isolate the interconnect surface by oxidation or surface activation were inconclusive but further studies are recommended to characterize the surfaces and correlate to filler separation results. From an underfill composition perspective, a lower filler content appears to increase filler separation, possibly because of an increased filler mobility at lower loading levels. Finally, it was demonstrated that assembly parameters believed to be of potential influence to underfill behavior, such as the chip join flux material, the post chip join cleaning process and the underfill capillary flow process, do not appear to impact the degree of filler separation from the resin matrix in the Cu-pedestal area.

To assess package robustness in the presence of this filler separation mechanism, a large die on organic substrate test vehicle with Cu-pedestal and SnAg solder interconnects was assembled and submitted to 2000 cycles of -55 to 125C deep thermal cycling. No electrical fails and no package related defects were observed on all modules submitted to this temperature cycling stress extension, which extends by a factor of two the qualification requirements. These reliability results corroborate the absence of field failure on multiple technology nodes using this underfill.

FEM was utilized to explain the stress results. It was demonstrated that the calculated stress field in the presence of filler separation at the Cu-pedestal is slightly higher but not significantly different from a control module with a uniform filler dispersion. This FEM calculation conclusion combined with the high underfill material adhesion and toughness as well as the appropriate manufacturing surface treatments, support the high reliability performance of the present evaluation as well as several other high-end, high-stress packages produced and investigated at IBM.

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