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Vapor Pressure Development in a FR4-Cu Composite Structure During Solder Reflow

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Abstract. This article presents a study on the development of vapor pressure a FR4-Cu composite structure when heated to a solder reflow temperature of 215 °C. Abaqus® finite element software was used to develop a representative two-dimensional model of the composite structure and to simulate moisture absorption and desorption processes. Simulation of transient moisture absorption was performed to predict moisture concentration distribution in the structure after being pre-conditioned in 85°C/85 % RH environment for 15 days. Simulation of transient moisture desorption was carried out at the solder reflow temperature to predict the redistribution of the moisture. Results of the moisture desorption simulation were used to compute magnitude of the vapor pressure in the structure. It was found that the moisture redistributes itself during the solder reflow process. Moisture concentration in the vicinity of the FR4-Cu interface, below the longer copper trace increases during the solder reflow. The vapor pressure in nearly 70 % of the FR4 material and close to the FR4-Cu interface, below the longer copper trace is almost equal to the saturation pressure of vapor at 215 °C. Distribution of the vapor pressure is very similar to the new distribution of moisture concentration resulting from moisture desorption process.

Introduction

During a solder reflow process of surface mounting components, an electronics package is typically heated up to 230°C to melt the solder material. Any moisture that was absorbed by the package during packaging process and storage will turn into vapor and exerts a pressure on interfaces between different materials within the package. The vapor pressure coupled with thermal stress resulting from thermal expansion coefficient mismatch could result in a structural failure often referred to as "popcorn" cracking. JEDEC standard [1] is widely used as reference for carrying out reliability test on moisture sensitivity of electronic packages. In a typical test the package is first pre-conditioned at certain temperature-humidity condition to allow the package to absorb some moisture. The amount of moisture absorbed by the package prior to solder reflow process was found to have strong influence on the susceptibility of the package to popcorn cracking. Kitano's [2], through his experimental work has shown the importance of local moisture concentration on popcorn failure of electronics package. This finding has highlighted the need for detail modelling of the moisture diffusion process in the electronics packaging as well as accurate estimation of the vapour pressure in the package during the reflow soldering process. The experimental and simulation studies of the popcorn cracking phenomenon in electronic packages have been performed by many researchers. One or two-dimensional finite element analysis of moisture diffusion have been employed. However, the procedure for estimating the magnitude and distribution of vapor pressure during the solder reflow process was not well established. J.H. Lim *et.al* [3] employed an ideal-gas relation between vapor pressure and the accumulated moisture content to calculate the vapor pressure generated in the electronics package during the solder reflow process.

Andrew A. 0. Tay [4] described two-dimensional finite-element simulations of the heat transfer and moisture diffusion in a small outline J-leaded (SOJ) package during moisture absorption, desorption and vapor pressure reflow process. They also used the ideal-gas relation to determine the moisture distribution and compute the vapor pressure developed in the package. J. E. Galloway [5] presented a finite element simulation of the moisture weight gain or loss in plastic ball grid array (PBGA) packages as a function of time. They employed the relationship between moisture solubility and the partial pressure of vapor to compute the weight gain by the package and the local moisture concentration in the package during a pre-conditioning process. T.Y. Tee and Z. Zhong [6] established a comprehensive and integrated package stress model for quad flat non-lead (QFN) package with detailed considerations of effects of moisture diffusion, heat transfer, thermo-mechanical stress, hygro-mechanical stress and vapor pressure induced during the solder reflow. They employed a representative volume element approach to estimate the vapor pressure generated inside the package. E.H. Wong *et.al* [7] introduced a new physical quantity, namely wetness fraction to overcome the vapor concentration discontinuity in the application of Fick's diffusion equation to multi-material systems. This enables the use of commercial thermal diffusion software to model the transient moisture diffusion phenomenon in an integrated circuit (IC) packaging. The wetness fraction approach is interesting because it provides a simple means of computing the vapour pressure in the package when its temperature is elevated up to 230°C during the reflow solder process. This new approach was bench marked against published works and found to corroborate remarkably well despite its simplicity. Kirsten Weide-Zaage *et.al* [8] carried out experimental investigation and two-dimensional finite element simulation of moisture absorption in a printed circuit board (PCB) when the board was exposed to 85°C/85% RH pre-conditioning environment. The effect of various arrangements of the copper layers on the distribution of moisture concentration in the board was also investigated.

There are not many studies in the literatures reporting the use of finite element method to simulate vapor pressure development in the PCB during the solder reflow process. So in this paper we present a study on the use of finite element method to simulate the development and estimate magnitude of vapor pressure in a simple FR4-Cu composite structure, representing a PCB, when it is heated to a solder reflow temperature of 215°C. General purpose finite element software was used to build a two-dimensional plane strain model of the FR4-Cu structure. An FE simulation of transient moisture absorption process was performed to predict the distribution of moisture in the structure after it was pre-conditioned in an 85 °C/85 % RH environment for a period of 15 days. Then an FE simulation of transient moisture desorption at during a solder reflow process at a peak temperature of 215°C was performed to predict the new distribution of moisture in the structure. The results obtained from the simulation of moisture desorption were used to estimate magnitude and distribution of the vapor pressure developed in the structure at the peak solder reflow temperature using a wetness fraction approach. The finite element model was validated by comparing results of similar FE analysis on a QFN package reported by T.Y. Tee and Z. Zhong [6].

Transient Moisture Diffusion Processes

Moisture Absorption (Pre-Conditioning) Process. During an actual pre-conditioning process the electronic package is typically exposed to a controlled temperature and humidity environment for certain period of time. As a result moisture is absorbed by the package and its amount is usually estimated by weighing the package at regular time intervals. At the temperature and pressure experienced by the package during the pre-conditioning process, the transient moisture diffusion phenomenon within the package is described by *Fick's* law, given by

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) \tag{1}$$

where C is local moisture concentration and D is moisture diffusivity which measures the rate of moisture diffusion within the structure. The moisture diffusivity D is given by

$$D = D_o \exp\left(\frac{-Q}{RT}\right) \tag{2}$$

where D_0 is diffusion coefficient, Q is activation energy (eV), R is Boltzmann constant ($R = 8.83 \times 10^{-5}$ eV/K), and T is absolute temperature (K).

The moisture concentration C is discontinuous across an interface between two different materials in a composite structure. This restricts the validity of the *Fick's* law with moisture concentration C as a field variable to homogeneous material structures only. However the discontinuity of moisture concentration can be eliminated by normalizing the local moisture concentration C with the saturated concentration C_{sat} of the respective materials [4]. That is,

$$w = \frac{C}{C_{sat}}; \qquad 1 \geq w \geq 0 \tag{3}$$

where w is called wetness fraction and C_{sat} is saturated moisture concentration, which represents the maximum amount of moisture that can be absorbed by a material at any given temperature and pressure. Its magnitude depends on the type of material, temperature, and humidity level. The lower limit of $w = 0$ means that the material is completely dry while the upper limit of $w = 1$ means that the material is saturated with moisture. Eq. (1) can then be written in terms of the wetness fraction w as,

$$\frac{\partial w}{\partial t} = D\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) \tag{4}$$

In general it is difficult to find analytical solution to the above differential equation. Fortunately, thermal diffusion analysis capability of commercial finite element software offers an opportunity for solving the *Fick's* diffusion equation in Eq. (4), by virtue of the similarity between these two diffusion equations. For thermal diffusion the corresponding differential equation is given by,

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) \tag{5}$$

where T is temperature, $\alpha = k/\rho c_p$ is thermal diffusivity of the material, which measures the rate of heat diffusion within the material, k is thermal conductivity and c_p is specific heat of the material.

Moisture Desorption (Solder Reflow) Process. During the solder reflow process in a surface mount technology (SMT) assembly an electronic package is often heated to an elevated temperature of up to 230°C. The moisture that was earlier absorbed by the package during storage or transportation will turn into vapor and it exerts pressure particularly on the interfaces between different materials in the structure. This thermally-induced vapor pressure coupled with thermal stress arising from the thermal expansion mismatch could result in an interfacial failure often referred to as a "popcorn" cracking [7]. Moisture desorption diffusivity is an important property of material especially during the solder reflow process. It is useful for estimating moisture weight loss from the material during such process. Since diffusivity D has a strong dependency on temperature, moisture desorption during reflow is generally a lot faster than moisture absorption during the pre-conditioning process.

Estimation of Vapor Pressure. The wetness fraction approach provides a relatively simple mean of estimating the magnitude of vapor pressure developed in a composite structure such as the electronic packages. Since *Fick's law* of diffusion is valid in gas, liquid, and solid, then the wetness fraction approach is also valid to be used in both the vapor and solid domains [7]. Since vapor can be assumed to behave like an ideal gas, we may write the wetness fraction

$$w = \frac{\rho_v}{\rho_{sat}} = \frac{P_v}{P_{sat}} \tag{6}$$

where ρ_v is vapor density, ρ_{sat} is saturated vapor density corresponds to the given temperature and humidity, P_v is vapor pressure and P_{sat} is saturated vapor pressure corresponds to that given temperature and humidity. From Eq. (6), the vapor pressure developed in the structure can be found by using

$$P_v = w \times P_{sat} \tag{7}$$

Eq. (7) can easily be implemented in the finite element model of the composite structure that we developed in this study to estimate the magnitude of the vapor pressure developed in the represented FR4-Cu structure, at the peak solder reflow temperature.

Finite Element (FE) Implementation

Figure 1 shows a two-dimensional plane-strain finite element model of FR4-Cu structure that represents a small portion of a printed circuit board (PCB), developed using Abaqus® software. It is 20 mm long and 3 mm height. Two thin copper traces which are 5 mm long (top) and 10 mm long (bottom), respectively were incorporated into the model. Both copper traces are of 3 mm thick and they represent copper "wires" that connect various surface mount components on the PCB. The model was meshed using four-node quadrilateral heat transfer elements for transient heat transfer simulations. A mesh sensitivity analysis was carried out to find out the number of elements that would minimize the effects of meshing density on the simulation results.

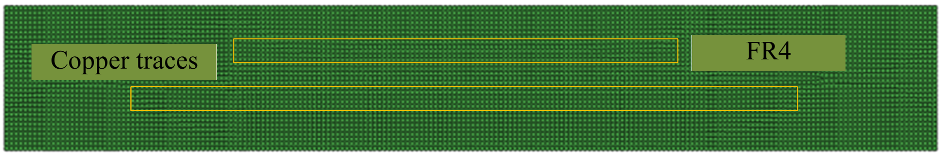


Figure 1 Two-dimensional FE model of FR4-Cu composite structure.

A transient thermal analysis was performed to simulate moisture absorption phenomenon during a pre-conditioning process in 85 °C/85 % RH environment for a period of up to 20 days. The wetness fraction approach described above was adopted during the simulation. The Abaqus finite element software does not have the required features for simulating moisture diffusion. The wetness fraction approach described above allows us to use a thermal-moisture analogy to overcome this limitation. In this case, we used transient heat diffusion analysis to simulate the moisture diffusion process in the composite structure. To perform the analysis, we first established a parametric similarity between transient heat diffusion and transient moisture diffusion process, as shown in Table 1.

Table 1 Parametric similarity for thermal-moisture analogy

Properties	**Thermal**	**Moisture**
Field variable	Temperature, T	Wetness fraction, w
Density	ρ (kg/m^3)	1
Conductivity	k (W/m ^{o}C)	$D*C_{sat}$ (kg/s m)
Specific Heat	C (J/kg ^{o}C)	C_{sat} (kg/m^3)

To perform the transient thermal analysis, the following boundary and initial conditions were prescribed on the model. All exterior surfaces of the structure were assumed initially saturated with moisture at the beginning of the pre-conditioning process while the interior of the structure was completely dry. Hence we prescribed wetness fraction of $w = 1$ at all nodes along the exterior surfaces and $w = 0$ at all the interior nodes of the finite element model. The copper traces acts as diffusion barriers, hence we set its diffusivity D equals to 0 for them. The total time for the simulation was set for the duration of 20 days. The material properties assigned to both the copper and FR4 are shown in Table 2.

Table 2 Properties assigned to copper and FR4 for moisture absorption simulation

Properties	**copper**	**FR4**
Density (kg/m^3)	1	1
Specific Heat (J/mol K)	1e-100	3.85
Conductivity (W/m K)	1e-100	5.814e-12

The finite element simulation of transient moisture desorption (during solder reflow process) was carried out in a similar manner as the moisture absorption described above. When a material that contains moisture is heated to an elevated temperature, some of the moisture will vaporize. The remaining moisture would rearrange itself within the material. The goal of this simulation is to predict the new distribution of the moisture in the FR4-Cu structure when it is heated to a solder reflow temperature of 215 °C. To achieve this, we prescribed different set of boundary and initial conditions on the finite element model. The exterior surfaces of the structure were assumed completely dry at the beginning of the solder reflow process. Hence we prescribed a wetness fraction of $w = 0$ on all nodes along the exterior surfaces of the finite element model. The result of the previous moisture absorption simulation was used as the initial condition. The moisture diffusivity D was evaluated at the solder reflow temperature of 215°C. Its value was found to be nearly a hundred times larger than the corresponding value for the moisture absorption simulation. The total time for the finite element simulation was set at 2 minutes. The material properties assigned to copper and FR4 are shown in Table 3.

Table 3 Properties assigned to copper and FR4 for moisture desorption simulation

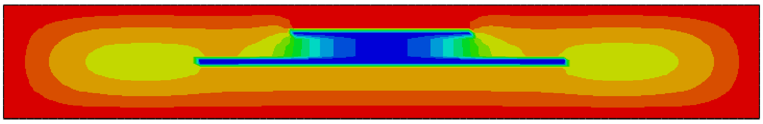
Properties	**copper**	**FR4**
Density (kg/m^3)	1	1
Specific Heat (J/mol K)	1e-100	3.85
Conductivity (W/m K)	1e-100	3.9142e-10

With the wetness fraction approach, the magnitude of vapor pressure developed in the structure at the solder reflow temperature of 215°C can easily be computed using the relation given by Eq. (7). The distribution of the vapor pressure within the structure will depend directly on the new distribution of the moisture concentration at this temperature.

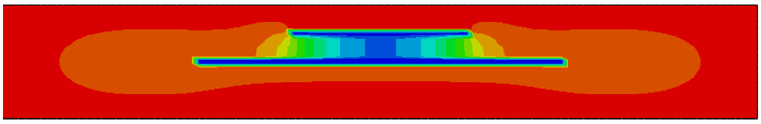
Results and Discussion

Moisture Absorption during Pre-Conditioning. Figure 2 shows distribution of moisture within in the composite structure during pre-conditioning in a 85 °C/85 % RH environment after 5, 10, 15 and 20 days, respectively. It can be observed that after 5 days, the FR4 material near the exterior surfaces is saturated with moisture (wetness fraction, $w = 1$). The same occurs in the area above the shorter copper trace. But the area between the two copper traces remains relatively dry. This is because the copper trace has blocked the moisture from diffusing into the region. The concentration of moisture appears to decrease gradually towards the interior region of the FR4 where it is seen to be about 50% dry. After 10 days, the saturated region of the FR4 grows bigger as more moisture was absorbed. The area between the copper traces can now be seen to be less dry. The distinct variation in moisture concentration within the FR4 can be seen clearly. After 15 days, the saturated area of the FR4 has grown even larger. The FR4 between the two copper traces is now about 15% dry. Finally, after 20 days of pre-conditioning, the FR4 appears to be entirely saturated with moisture while the region between the two copper traces is getting a lot more wet. These findings suggest that when exposed to a very damp environment, an FR4 material does has the ability to absorb moisture. Depending on the dimension of the structure and the length of exposure, there is a possibility that the material would eventually become saturated with moisture.

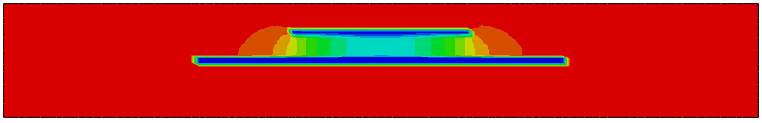
(a) After 5 days of pre-conditioning



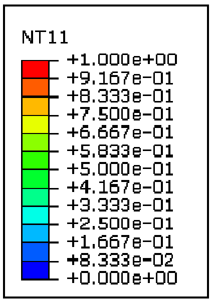
(b) After 10 days of pre-conditioning



(c) After 15 days of pre-conditioning



(d) After 20 days of pre-conditioning



Wetness fraction,
$w = C/C_{\mathrm{sat}}$

FIGURE 2 Distribution of moisture concentration during the pre-conditioning process.

Moisture Desorption during Solder Reflow. Figure 3 shows the result obtained from the moisture desorption simulation. It corresponds to the initial distribution of moisture in the structure after 15 days of pre-conditioning (Figure 3(a)). Note that for the moisture desorption process at the solder reflow temperature of 215 °C, the moisture diffusivity D was found to be 3.9142 x 10^{-10} m^2/s. This shows that the rate of moisture desorption is approximately a hundred times faster than the rate of moisture being absorb by the material. Figure 3(b) shows the new moisture distribution at solder reflow temperature of 215°C. The entire exterior surfaces are completely dry due to the prescribed boundary condition of zero moisture. In actual condition the moisture at the exterior surfaces would almost immediately evaporate as the structure is heated and held at 215°C for certain duration. This creates moisture concentration gradient within the structure which causes the moisture to redistribute itself. As seen from the figure the FR4 is now about 70% saturated with moisture and nearly 50% of the FR4-copper interface, below the longer copper trace, is saturated with moisture. The moisture distribution between the two copper traces does not seem to be much affected by the reflow temperature.

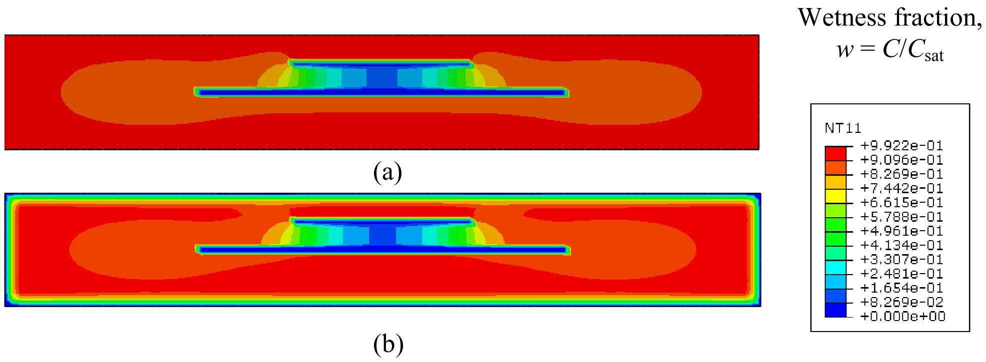


FIGURE 3 (a) Distribution of moisture after 15 days of pre-conditioning. (b) The new distribution of moisture at a temperature of 215°C during solder reflow process.

Development of Vapor Pressure. During the solder reflow process any moisture trapped in the material would transform into vapor that exit static pressure called the vapor pressure. Figure 4 shows the distribution of the vapor pressure, P_v (in Pascal) at a temperature of 215°C during the process. The magnitude of the vapor pressure was estimated during the finite element simulation using Eq. (7), in which the saturation pressure of water vapor at 215°C was taken to be 2.4 MPa. It can be observed that distribution of the vapor pressure is similar to that of the moisture shown in Figure 3(b). A zero vapor pressure condition occurs on the entire exterior surfaces and a gradient of vapor pressure occurs in the FR4 close to the exterior surfaces. The magnitude of vapor pressure in nearly 70% of the FR4 is close to the saturation value of 2.4 MPa. The same occurs at nearly half of the FR4-copper interface below the longer copper trace. At the left and right of the longer copper trace the vapor pressure in the FR4 is about 2 MPa. Between the two copper traces the vapor pressure varies from about 0.3 to 1.8 MPa. If the magnitude of the vapor pressure at the FR4-Cu interfaces is greater than the bonding strength at these location, there could be a possibility of interface delamination, a failure popularly known as the “popcorn cracking” in the structure.

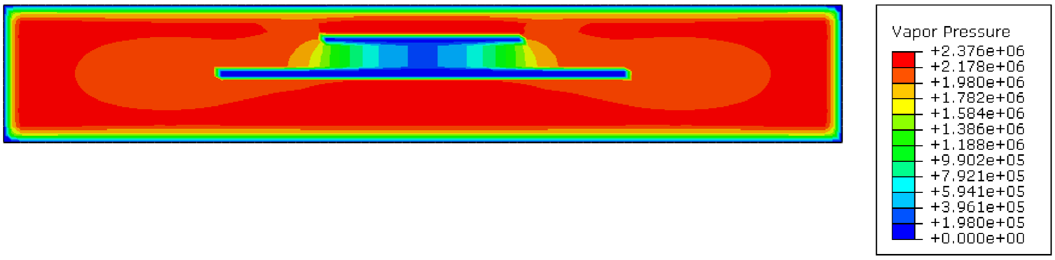


FIGURE 4 Distribution of vapor pressure P_v (in Pascal) at solder reflow temperature of 215°C.

Validation of the Finite Element Model. The finite element model we developed in this work was validated by comparing our simulation results with the results of similar work reported by T.Y. Tee *et.al.* [6]. They performed finite element simulations of transient moisture absorption in a quad flat no-lead (QFN) electronics package structure. Figure 5 shows the distribution of moisture (represented by wetness fraction *w*) in a two-dimensional half-model of the package, after pre-conditioning and during solder reflow processes. We developed a similar finite element model of the package and performed the same simulations with similar material and thermal properties, and imposed the same boundary conditions on the model. Figure 6 shows the distribution of moisture in the package we obtained from our simulations. It can be observed that the trend of moisture distribution after 1 hour and 12 hours of pre-conditioning are in very good agreement with those reported by T.Y. Tee *et.al.* [6]. The new distribution of moisture in the structure during solder reflow process also seem to agree very well with that reported by the author. Hence, we conclude that the finite element model of a simple FR4-Cu structure we developed in our study and the transient heat transfer analogy we adopted for simulating both moisture absorption and desorption are valid to be used in our study.

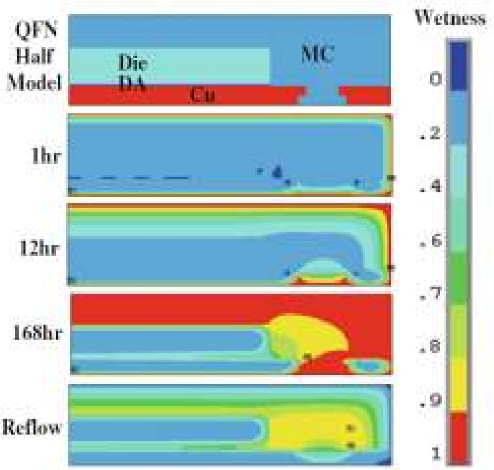


FIGURE 5 Distribution of moisture (represented by wetness fraction, *w*) in a QFN package reported by T.Y. Tee *et.al.*[6].

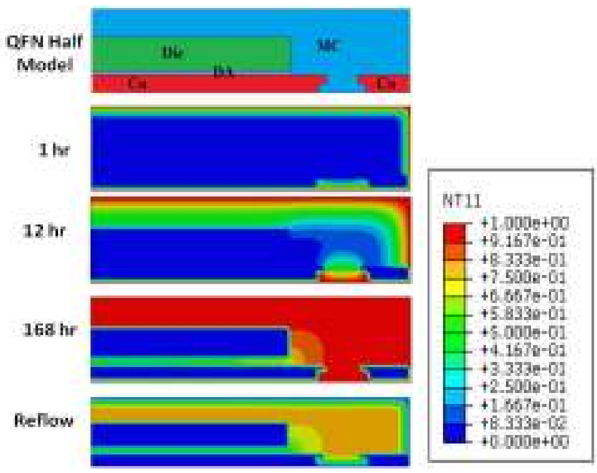


FIGURE 6 Distribution of wetness fraction *w* in the QFN package we obtained using the FE methodology developed in this study.

SUMMARY

A finite element model for predicting development of vapor pressure in a simple FR4-copper composite material at a solder reflow temperature of 215°C was developed in this study. Transient simulation of moisture absorption was carried out to predict the distribution of moisture in the structure after pre-conditioned at an 85°C/85%RH environment for up to 20 days. Simulation of transient moisture desorption was performed to predict new distribution of moisture in the structure at peak solder reflow temperature of 215°C. It was found that after 15 days of pre-conditioning the FR4 is nearly 80% saturated with moisture. The moisture redistributes itself at the peak solder reflow temperature as some of it being desorbed. The distribution of vapor pressure in the FR4 at the peak solder reflow temperature is similar to the new distribution moisture at that temperature. The magnitude of the vapor pressure in nearly 70% of the FR4 and at the FR4-copper interface below the lower copper trace is closed to the saturation pressure of water vapor.

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