

# A Comparison of the Theory of Moisture Diffusion in Plastic Encapsulated Microelectronics With Moisture Sensor Chip and Weight-Gain Measurements

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**Abstract**—In this paper, the issues pertaining to moisture diffusion in PEMs are explored and discussed. The existing models of moisture diffusion in plastic molding compounds and PEMs are reviewed. Results, modeling and analysis of moisture sorption experiments performed in this study are presented. The moisture sorption experiments were conducted on a set of PEM samples with a common type of encapsulant material to

- 1) characterize sorption behavior;
- 2) compare weight gain measurement to the measurement of moisture concentration using a moisture sensor device at the die surface;
- 3) assess the moisture sensor measurement method.

In the case of PEM samples tested in this study, simple Fickian diffusion was shown to agree closely with the experimental results. In one case, a relatively small anomaly from Fickian diffusion was observed and was attributed to swelling and relaxation phenomena at later stages of moisture sorption in the molding compound. The calibration constants determined for the sensors in this study were found to be significantly different from those collected by the manufacturer prior to the encapsulation of the devices. This problem is believed to be degradation in sensitivity of the moisture sensor due to exposure to high temperatures and storage conditions.

**Index Terms**—Capacitance change, Fickian diffusion modeling, hydrogen bonding, moisture diffusion, moisture sensor, plastic encapsulated microelectronics.

## I. INTRODUCTION

PLASTIC molding compound has become the leading packaging material in today's microelectronic packaging industry. Lower design and manufacturing costs, higher productivity, and improved part reliability are some of the

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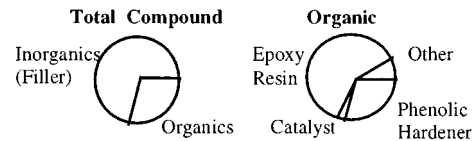


Fig. 1. Molding compound composition.

advantages of the plastic encapsulation over its hermetic counterpart [1].

The plastic molding compounds used in electronic packaging consist of resin, hardener, filler and other materials (Fig. 1) [2]. The common resin used is Epoxy Cresol Novolac (ECN). The common hardener and filler used are phenolic novolac (PN) and fused silica (FS), respectively.

A disadvantage of plastic molding compounds is that they are hydrophilic [3] and absorb moisture when exposed to a humid environment. Moisture in PEMs can lead to many reliability problems such as cracking, de-adhesion, and corrosion of the metallization. These reliability problems can occur both during and after the manufacturing process.

One common problem associated with moisture occurs during the soldering of the surface mount package to the printed wiring board and is referred to as "popcorning." PEMs can absorb moisture during storage prior to soldering. During solder reflow, the surface mount packages are subjected to high temperatures (i.e., 215 °C) in a relatively short time. The rapid heating causes the moisture at the delaminated interface between the die-pad, or the top of the die, and the molding compound to vaporize and it creates a high build-up of pressure at the interface. The pressure causes bulging at the interface and eventually the package cracks [4], [5].

Another problem associated with moisture is the corrosion of the metallization in PEM. Corrosion of the metallization on the die can lead to electrical degradation and eventually to a short or open circuit [6].

Prediction and prevention of the problems associated with moisture in PEMs, requires understanding and modeling of the moisture diffusion behavior in plastic molding compounds and PEMs. This paper presents modeling of moisture diffusion in PEMs using two types of measurements: package weight gain to determine moisture content, and capacitance measurements to determine moisture concentration at the die surface. Some concerns with the capacitance measurement method are also presented.

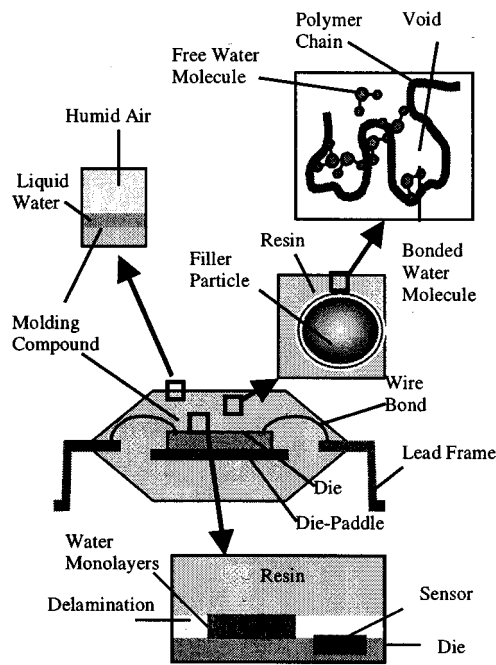


Fig. 2. Moisture diffusion in PEM.

## II. MOISTURE DIFFUSION THEORY

Moisture diffusion in PEMs is not a simple process (Fig. 2) and there are many issues associated with it. One issue is the phase of the water molecules during sorption into the plastic package. For consistent terminology throughout this paper, we will use “water” and “moisture” interchangeably for  $H_2O$  molecules in any phase. In a typical environment to which PEMs are exposed, water molecules may be present in the forms of vapor, liquid or both. Moisture can transport through the molding compound, also in the forms of liquid [7], vapor or both [8]. Moisture sorption may also involve phase transformation. Water vapor from the ambient may condense to the liquid phase at the exposed surfaces of the plastic package [9] or in the voids in the molding compound or delaminated areas inside the package [8], [9]. The condensed moisture can be either in the form of discrete droplets on the surface or in the form of uniform layers. These water layers are often quantified in terms of monolayers. Some studies have estimated the number of monolayers of water necessary to initiate and support corrosion of the metallization in PEMs [9].

A second issue related to moisture sorption, is the path of diffusion. Moisture mainly diffuses through the molding compound, but a small portion can also diffuse through the interfaces between the molding compound and other materials (i.e., leads), if there is de-adhesion at their interfaces. Separation of the molding compound from adjacent materials in PEMs can occur from stresses due to CTE mismatch during heating and cooling, or from a decrease in adhesion strength at the interfaces due to moisture, or from combination of both. Inside the molding compound, the moisture may diffuse through the polymeric resin or through the filler–resin interface (if there is separation between filler and resin). The diffusion through the polymeric resin can be referred to as “bulk diffusion” and the diffu-

sion through interfaces between polymeric resin and other materials (i.e., leads, lead-frame and fillers) can be referred to as “interfacial diffusion.”

A third issue pertaining to moisture diffusion, is the interaction between the water molecules and the polymer chains in the polymeric resin. Water molecules in the polymeric resin, can either diffuse freely through the “free volume,” or form hydrogen bonding to the polymer chains. The “free volume” of the polymeric resin is defined as the volume of the resin without the volume of the polymer chains and the volume due to thermal vibrations of the polymer chains.

A fourth issue to consider in moisture sorption of molding compound samples is the thickness issue. For relatively thin samples, moisture sorption can be considered one-dimensional. In other words, the moisture is considered to diffuse predominantly through the larger surfaces of the samples, and diffusion through the edges is considered negligible. As the thickness of the block or PEM samples increases, moisture diffusion through the edges may become more significant.

Nevertheless, there are engineering advantages (i.e., lower cost and time efficiency) to quickly assessing moisture diffusion properties of PEMs such as the rate of moisture sorption and saturation moisture content at given environmental conditions.

Moisture diffusion in plastic molding compound samples or PEM packages is commonly modeled using one-dimensional Fickian equation [10]–[14]. In this study, the packages under testing were relatively thin, therefore, moisture diffusion through the edges was assumed negligible and diffusion was modeled using a one-dimensional Fickian model. For relatively thicker samples (block samples), diffusion can be more accurately simulated using three-dimensional (3-D) Fickian models and finite element methods [8], [15]. Diffusion coefficient can be calculated by minimizing the difference between the experimental weight gain data and the 3-D Fickian moisture diffusion model. Galloway *et al.* [15] used 3-D FEM model to predict moisture gain and local moisture concentration for a specific PBGA package.

Finite element method modeling of moisture diffusion in PEMs has the advantage of considering complex geometries that are not easily solvable using analytical techniques. Also, geometry effects such as internal vias and metallization on the die pad can be included [15].

While finite element modeling may provide a more accurate analysis of moisture diffusion in PEM as compared to 1-D analysis or use of 3-D analytical solutions for simplified geometry, it also has disadvantages in terms of cost and time.

In addition to Fickian models, there are other models such as ‘dual mode sorption’ model [11] and quasisteady state (QSS) models [9]. The “dual mode sorption” model is based on the fact that water molecules in the molding compound exist in two states: bound to the polymer chain and unbound. The QSS model is a simpler model compared to the full transient Fickian model and is used for the general case of enclosure with a finite size cavity. In the case of moisture diffusion in plastic microelectronic packages, the full transient Fickian model gives a more accurate prediction.

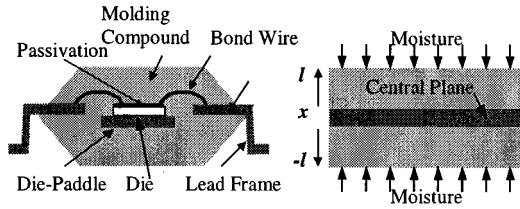


Fig. 3. Modeling the plastic package as a plane sheet of thickness  $2l$ , with an impermeable central plane.

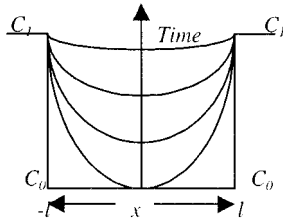


Fig. 4. Boundary conditions.

Fick's law [16] for one-dimensional diffusion is

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (1)$$

where  $C$  is the concentration of the diffusing substance,  $t$  is the time,  $D$  is the diffusion coefficient, and  $x$  is the axis along the concentration gradient.

#### A. Initial and Boundary Conditions

Typical PEMs such as plastic quad flat package and dual in-line packages can be modeled as a plane sheet of thickness  $2l$  ( $2l$  is the thickness of package minus the thickness of the die and die-paddle). Both surfaces are assumed to be at a constant concentration  $C_1$  with initial uniform concentration  $C_0$  in the region of  $-l < x < l$  and an impermeable central plane (Fig. 3).

An impermeable central plane imposes a zero concentration gradient. The same condition exists at the central plane of a plane sheet with symmetrical initial and boundary conditions (Fig. 4). The initial and boundary conditions can be stated as

$$\begin{aligned} C &= C_1, & x &= -l, & x &= l, & t &\geq 0 \\ C &= C_0, & -l < x < l, & & t &= 0 \\ \frac{\partial C}{\partial x} &= 0, & x &= 0, & t &\geq 0. \end{aligned} \quad (2)$$

#### B. Simple Diffusion

Simple diffusion is a process in which no chemical reaction or bonding of the diffusing substance occurs and is described by (1). Upon solving Fick's diffusion equation using the method of separation of variables, the concentration distribution is expressed as [16]

$$\frac{C - C_0}{C_1 - C_0} = 1 - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \exp(-At) \cos(Bx) \quad (3)$$

where  $A = D(2n+1)^2\pi^2/4l^2$ ,  $B = ((2n+1)\pi)/2l$  and  $C$  is the concentration of moisture at distance  $x$  and time  $t$ . The total

amount of moisture  $M_t$  that has entered the sheet at time  $t$  is given by

$$M_t = \int_{-l}^l (C - C_0) dx. \quad (4)$$

Integrating the above equation and defining  $M_\infty$  as the moisture in the sheet after infinite time (equilibrium moisture), the following expression is derived:

$$\frac{M_t}{M_\infty} = 1 - \sum_{n=0}^{\infty} \frac{8}{(2n+1)^2\pi^2} \exp(-At) \quad (5)$$

where  $A = D(2n+1)^2\pi^2/4l^2$ . The corresponding equation, useful for small times, is

$$\frac{M_t}{M_\infty} = 2 \left( \frac{Dt}{l^2} \right)^{1/2} \left\{ \pi^{-1/2} + 2 \sum_{n=1}^{\infty} (-1)^n \operatorname{erfc} \frac{nl}{\sqrt{Dt}} \right\}. \quad (6)$$

The diffusion coefficient,  $D$ , of a plane sheet of thickness  $l$  can be calculated using

$$\frac{M_t}{M_\infty} = 4 \left( \frac{Dt}{\pi l^2} \right)^{1/2}. \quad (7)$$

#### C. Diffusion With Bonding

The water molecule is polar and is capable of forming hydrogen bonds with hydroxyl groups [7], [17], [18]. Water molecules can exist in polymeric media in two states: unbound, or bound to the polymer molecule groups [7], [19]. During moisture diffusion in plastic molding compounds, some of the water molecules may form hydrogen bonds with the polymer molecules and become immobilized, while other diffusing water molecules move freely through the voids in the plastic compound.

This phenomena has been addressed by "dual mode sorption theory" where the moisture concentration in the polymeric material consists of the concentration of moisture diffusing in the holes,  $C_H$ , and the concentration of moisture dissolving in or associating with the polymeric matrix,  $C_D$

$$C = C_H + C_D \quad (8)$$

and  $C_H$  is expressed as

$$C_H = \frac{C_H^* bp}{1 + bp} \quad (9)$$

and  $C_D$  is expressed as

$$C_D = kp \quad (10)$$

where  $C_H^*$  is the hole saturation constant,  $b$  is the hole affinity constant,  $p$  is the equilibrium pressure, and  $k$  is Henry's law constant [11].

Diffusion in plastic molding compounds and packages, however, has been shown to follow simple Fickian diffusion [10]–[14], [20]. There is an alternative approach in addressing dual mode moisture sorption in plastic compounds while using the Fickian diffusion model.

If the bonding of the water molecules to the polymer chains occurs very rapidly relative to the diffusion process, then it is considered instantaneous. The concentration  $S$  of bonded water molecules is assumed to be proportional to the concentration  $C$  of free water molecules and it is expressed as

$$S = RC \quad (11)$$

where  $R$  is a constant. The diffusion equation is modified as

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - \frac{\partial S}{\partial t}. \quad (12)$$

Upon substituting (8) in (9), the diffusion equation becomes

$$\frac{\partial C}{\partial t} = \frac{D}{R+1} \frac{\partial^2 C}{\partial x^2}. \quad (13)$$

The solutions to moisture diffusion with bonding in PEMs are the same as in simple moisture diffusion given the same initial and boundary conditions as stated in expressions (2a,b,c).

In this case,  $D/(R+1)$  is the modified diffusion coefficient. Therefore, the overall process of moisture diffusion with bonding is slower than for simple diffusion process.

Bonding of water molecules to the polymer chains can cause swelling [7] and relaxation of the polymeric material. A model that addresses this issue is expressed as [11]

$$\frac{M_t}{M_\infty} = 1 - \left[ 1 - \frac{k_0 t}{C_0 \left(\frac{l}{2}\right)} \right]^n \quad (14)$$

where  $M_t$  is moisture content at time  $t$ ,  $M_\infty$  is saturation moisture content,  $k_0$  is a relaxation constant,  $C_0$  is the equilibrium solubility parameter,  $l$  is the sample thickness. For a slab the exponent  $n$  is equal to one and the percent moisture content is proportional to time.

#### D. Equilibrium Moisture Concentration at the Die Surface

At the die surface, the equilibrium (or saturation) moisture concentrations of the molding compound, air (if delaminated), and moisture sensor on the die are related by Henry's law constants

$$C_{\text{mold @ die}} = K_m C_{\text{air}} \quad (15)$$

$$C_{\text{sensor}} = K_s C_{\text{air}} \quad (16)$$

$$C_{\text{air}} = C_{\text{ambient}} \quad (17)$$

where  $K_m$  and  $K_s$  are the Henry's law constants.

In this study, we assume an infinitesimal delamination at the interface of the die and the molding compound. Therefore, the saturation moisture concentration in the moisture sensor is the same as the ambient moisture concentration.

#### E. Diffusion and Molding Compound Characteristics

Moisture diffusion in molding compounds is related to molding compound characteristics, in particular, the molecular sized voids in the polymer structure and the polymer-water affinity. The molding compound characteristics are functions of polymer structure, polymerization process, mold process, curing, and post-curing [20].

TABLE I  
STANDARD MOLDING AND POST MOLD CURE CONDITIONS

Characteristics	Package 1 EME-6300	Package 2 EME- 7320CR
Transfer Pressure	70(kgf/cm <sup>2</sup> ) 50-100	85(kgf/cm <sup>2</sup> ) 70-120
Mold Temperatures	175(°C) 170-180	180(°C) 175-185
Cure Time	90(sec) 70-120	45(sec) 40-60
Post-Mold Cure Temp	175(°C) 165-180	175(°C) 170-180
Post-Mold Cure Time	4(hours) 4-10	8(hours) 4-10

The moisture diffusion behavior observed in this study can be applicable to those packages with molding compounds of the same type of polymer structure, molding process history, and curing and post-curing treatment.

Molding and post mold cure conditions for the encapsulant materials used in packages tested in this study are presented in Table I. Both types of the molding compounds were manufactured by Sumitomo. Type 1 and Type 2 packages were encapsulated with EME-6300, and EME-7320CR molding compounds, respectively. The values presented in Table I are standard values and they may be subjected to slight variation due to the variability in the processing conditions. Ranges of the actual processing conditions are also included in Table I.

### III. EXPERIMENTS

Two types of experiments were conducted: weight gain measurements and capacitance measurement at the die surface. Two types of samples were tested; three samples from Type 1 and four samples from Type 2. Type 1 and Type 2 samples have different moisture sensor chips, NAT-01 and ACT5.0, respectively.

#### A. Weight Gain Measurements

Weight gain measurements were performed to measure the moisture content in the whole package. The bulk moisture content was determined from the following expression:

$$M\% = \frac{W_{\text{wet}} - W_{\text{dry}}}{W_{\text{dry}}} \times 100 \quad (18)$$

where  $W_{\text{wet}}$  is the weight of the sample that has absorbed moisture,  $W_{\text{dry}}$  is the weight of dry sample, and  $M\%$  is the percent moisture content.

Packages were dried initially at 125 °C for 24 h or more until no further weight loss was detected. The packages had dimensions of 2 × 7 × 13 mm. The packages were weighed using a Mettler analytical balance and Perkin Elmer AD-6 Auto-balance, both with a resolution of 0.1 mg. The packages were then exposed to selected condition in the humidity chamber. Both Type 1 and Type 2 packages were exposed to 85 °C/85% RH for one week. Type 2 packages were also exposed to 35 °C/75% RH for three weeks. The packages were periodically removed and weighed and returned to the chamber for further soaking.

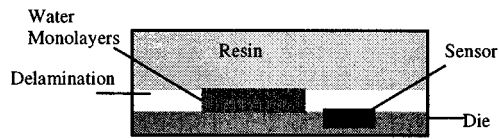


Fig. 5. Moisture at the die/molding compound interface.

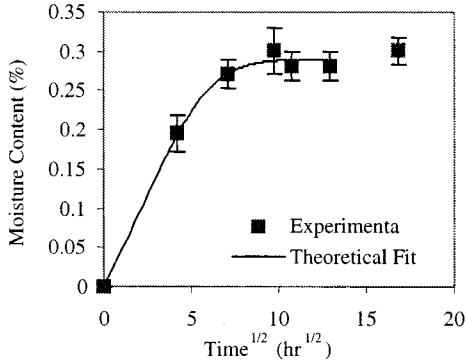


Fig. 6. Weight gain measurements of Type 1 packages subjected to 85 °C/85% RH.

### B. Capacitance Measurements

Capacitance measurements at the die surface were conducted using the Sandia MS test chips. Two types of MS test chips were used: NAT-01 and ACT5.0. Both test chips are 2.52 mm by 2.52 mm. The NAT-01 test chip contains two active porous Si moisture sensors, one passivated with 5000 Å of PECVD SiN, and the other unpassivated. The ATC5.0 contains a single unpassivated moisture sensor. Moisture sensors are constructed by anodizing lightly doped *p*-type wafers in an electrochemical cell that contains hydrofluoric acid. Films are approximately 1 μm thick and contain pore diameters in the range of 130 Å. These pores readily absorb moisture, initially as monolayers and later as liquid water, when exposed to increasing ambient moisture concentrations. The resulting change in dielectric constant of the film is detected as a shift in capacitance between the unanodized substrate and a 2 μm line and space Al grid formed on top of the porous Si film [21].

## IV. RESULTS AND DISCUSSION

The results from weight gain measurements and capacitance measurements were plotted and compared to Fickian modeling.

### A. Weight Gain Results

The plots of weight gain measurements versus  $\text{time}^{1/2}$  are shown in Figs. 5–7. Theoretical fit using Fickian equation (3) is also included in the figures for comparison. The moisture diffusion characteristics of the packages, namely the diffusion coefficient ( $D$ ) and the saturation moisture content ( $M_{\text{sat}}$ ) are presented in Table II. The diffusion coefficient was calculated using the reduced form of Fickian equation (7).

The moisture sorption in packages tested in this study follow Fickian diffusion. The small deviation from Fickian at the later stage of sorption of Type 2 at 85 °C/85% RH is probably due to relaxation of polymer chains and swelling. The water molecules while diffusing through the micro voids of the sample, maybe forming hydrogen bond with the polymer

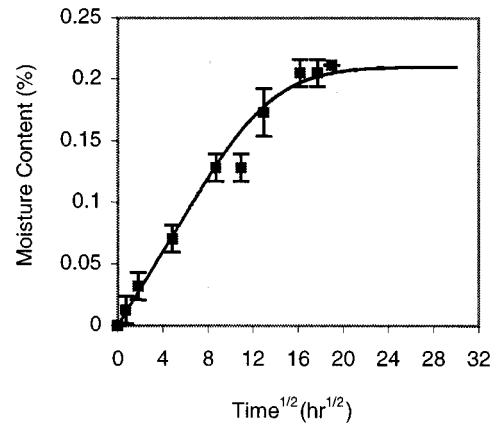


Fig. 7. Weight gain measurements of Type 2 packages exposed to 35 °C/75% RH.

TABLE II  
MOISTURE DIFFUSION CHARACTERISTICS

Type/ Condition	Value $D$ ( $\text{cm}^2/\text{s}$ )	$M_{\text{sat}}$ (%)
Package Type 1 85°C/85%RH	$3.8 \times 10^{-8}$	0.29
Package Type 2 35°C/75%RH	$7.5 \times 10^{-9}$	0.21
85°C/85%RH	$5.3 \times 10^{-8}$	0.39

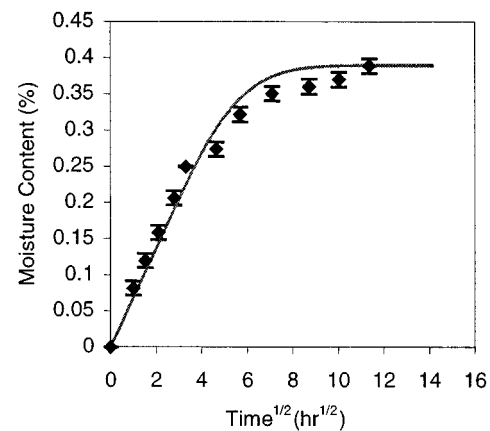


Fig. 8. Weight gain measurements of Type 2 packages exposed to 85 °C/85% RH.

chain and cause swelling. The water molecule immobilization plus the additional diffusion space due to swelling can lead to deviation from Fickian diffusion.

### B. Capacitance Results

The capacitance change with  $\text{time}^{1/2}$  at the unpassivated and passivated sections of the die surface is plotted in Fig. 8. The capacitance change at the passivated die surface is included in this figure for comparison. Die passivation appears to be an effective method of slowing down moisture sorption at the die surface.

The moisture concentration at the unpassivated die surface is calculated using Fickian diffusion equation (3) and the diffusion coefficient calculated from weight gain measurements. The plot of the theoretical moisture concentration and the capacitance measurements at the unpassivated die surface is shown in Fig. 9.

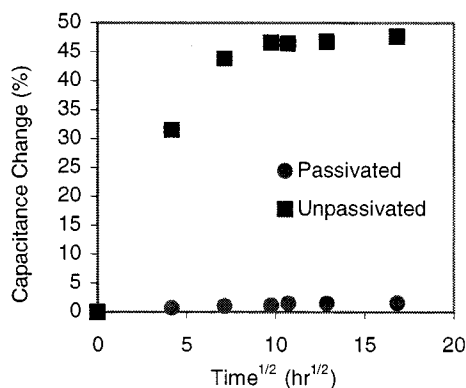


Fig. 9. Capacitance change due to moisture at the die surface in Type 1 packages subjected to 85 °C/85% RH.

TABLE III  
DECAY IN SENSITIVITY OF SANDIA NAT-01 MS CHIP AFTER EXPOSURE TO AIR AT 300 °C FOR 4 h

Condition/Days	$\Delta Cap (\%) / C^{1/2}$ ( $l/l$ )
Baseline	120
After Bake-out	113
10 Days	100
20 Days	78

The saturated concentration is 0.9 ( $l/l$ ) at 85 °C/85% RH. The relationship between the capacitance change ( $\Delta Cap\%$ ) and the square root of moisture concentration ( $C^{1/2}$ ) at the die surface can be approximated as linear [21] and can be expressed as

$$\Delta Cap (\%) = Cb \times C^{1/2} \left( \frac{l}{l} \right) \quad (19)$$

where  $Cb$  is the calibration ratio and its value is 50. The lower value of calibration constant of NAT-01 MS chip calculated in this study relative to those calculated at the Sandia National Laboratories, show decay in the original sensitivity of the MS chip (Table III). The decay in sensitivity of the MS chip is believed to be due to temperature exposures and ambient storage [21].

The plot of capacitance change and square root of moisture concentration calculated using the Fickian equation is shown in Fig. 10. The calibration ratio for the encapsulated ACT5.0 chip exposed to 35 °C/75% RH is 135. The calibration ratio for the encapsulated ACT5.0 chip exposed to 85 °C/85% RH is 64.

This study suggests that the capacitance measurement method cannot be used independently to measure moisture concentration at the die surface, if the moisture sensor was exposed to high temperatures and storage after the calibration ratio had been determined. This is due to the fact that the sensitivity of the moisture sensors decays upon exposure to high temperatures and storage. The decay in sensitivity of the moisture sensor results in overestimating the moisture concentration at the die surface up to two or three times its value.

The initial part of the capacitance curve (0 to 1  $h^{1/2}$ ) in Fig. 11 agree with the Fickian prediction of the moisture concentration at the die surface. This shows that upon subjecting PEMs to humid environment, although the moisture ingress into the molding compound is instantaneous, the die surface remains

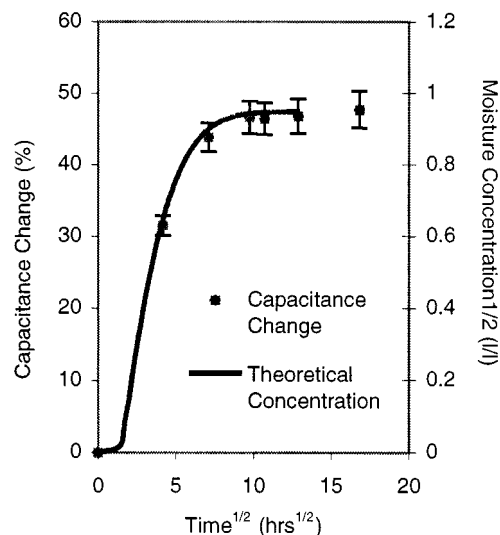


Fig. 10. Experimentally measured capacitance change and theoretically determined moisture concentration at the unpassivated die surface in Type 1 packages subjected to 85 °C/85% RH.

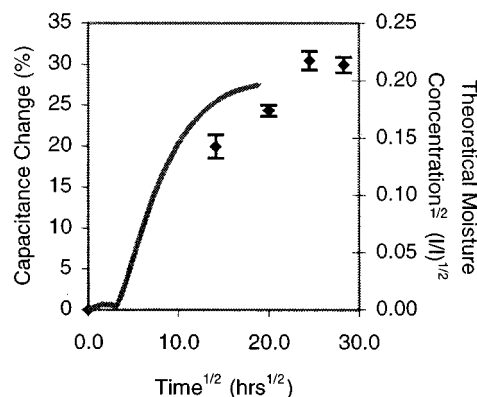


Fig. 11. Capacitance change due to moisture at the unpassivated die surface in Type 2 packages subjected to 35 °C/75% RH.

relatively dry for a small duration of time,  $t_{dry}$ , until moisture reaches the die. The  $t_{dry}$  for the packages subjected to 85 °C/85% RH was about 1 h.

The weight gain measurements and capacitance measurements follow Fickian diffusion. This suggests that the bonding of water molecules with polymer chains may be either less dominant compared to simple diffusion or the bonding is instantaneous. The slight deviation from Fickian behavior at a later stage in one sorption experiment reveals possible relaxation and swelling of polymer chains due to water molecule bonding.

The capacitance measurements, on the other hand, can be useful in evaluating moisture concentration at the die surface if conducted in conjunction with weight gain measurements. The capacitance measurement method produces the profile of the moisture concentration at the die surface, which independently validates the diffusion equation used for modeling the moisture sorption data collected from weight gain measurements (Fig. 12).

Upon calculating the calibration ratio from weight gain measurements and capacitance measurements, if exposure to the environment for relatively short time results in negligible decay in

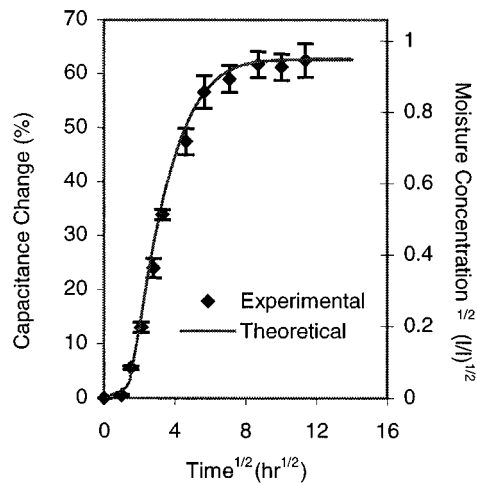


Fig. 12. Capacitance change due to moisture at the unpassivated die surface in Sandia packages subjected to 85 °C/85% RH.

sensitivity of the MS chip, the moisture sensor can be used independently to measure moisture concentration at the die surface at any given time.

## V. CONCLUSION

Two types of experiments were performed to determine moisture diffusion characteristics in Plastic Encapsulated Microelectronics. A one-dimensional Fickian simple diffusion model was used to calculate diffusion coefficient and model moisture sorption in PEMs. Capacitance measurements were performed and presented as an alternative experimental method for determining moisture concentration at the die surface. The results from capacitance measurements and weight gain measurements were compared with the moisture diffusion theoretical models.

The simple one-dimensional Fickian model was shown to closely agree with weight gain measurements and capacitance measurements. This study suggested that the capacitance measurement method cannot be used independently to measure moisture concentration at the die surface. This is due to the fact that the sensitivity of the moisture sensors decays upon exposure to high temperatures and storage.

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