Hermeticity Evaluation of Polymer-Sealed MEMS Packages by Gas Diffusion Analysis
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Abstract—A gas transport mechanism is studied to characterize the hermetic behavior of polymer-sealed microelectromechanical systems packages. Diffusion-based governing equations, which are fundamentally different from the conduction-based governing equations used for metallic seals, are proposed to predict a change in cavity pressure. An effective numerical scheme is developed to implement the governing equations. The validity of the governing equations is corroborated by the optical leak test. The verified gas diffusion model is utilized to investigate the effect of the diffusion properties and geometries of polymeric seals on the gas leak behavior.

Index Terms—Gas diffusion, gas leakage, hermeticity, microelectromechanical systems (MEMS) package, polymer seals.

I. INTRODUCTION

MICROELECTROMECHANICAL systems (MEMS) devices are ubiquitous. They are found in various fields such as medical diagnostics, communications, automobiles, etc. The most critical role of MEMS packaging is to provide an internal cavity for moving parts and to maintain the initial condition of the cavity. The cavity is produced by sealing a gap between cap and substrate wafers.

Hermeticity of the MEMS package is a measure of the ability to maintain an acceptable level of stable and sometimes inert ambient in the cavity. It impacts device reliability and, hence, lifetime expectancy. Poor hermeticity can lead to ingress of contaminants, ambient gases, and moisture thereby causing performance degradation. Good hermeticity is essential for compliance with performance and reliability standards.

The most commonly used sealing materials to provide hermeticity are low-melting point eutectics such as AuSn [1], AuSi [2], and other tin-based alloys [3]. More recently, polymers have gained widespread acceptance due to several advantages that they offer [4]; they include lower processing temperatures, compatibility with integrated circuit wafers, and the ability to compensate to some extent by the polymer adhesive [5]. Examples of polymeric seals include benzocyclobutene, parylene, polyimides, and negative photoresists [6], [7].

In metallic seals, gas leakage is attributed to randomly present defects (nanoscale leak channels). This gas conduction mechanism of metal-sealed MEMS packages has been studied and well understood by adopting the theories developed in the vacuum technology [8]–[16]. In polymeric seals, however, gas leakage occurs due to the inherently permeable nature of polymers (bulk material property). To the best of authors’ knowledge, this bulk diffusion mechanism has never been addressed properly for polymer-sealed MEMS packages.

This paper will focus on three objectives:
1) to propose gas diffusion mechanism-based governing equations for hermeticity evaluation of the polymer-sealed MEMS package;
2) to develop a numerical scheme to implement the governing equations;
3) to corroborate the validity of the governing equations.

In addition, the proposed modeling scheme will be utilized to gain an understanding of gas transport behavior in polymer-sealed MEMS packages, more specifically the effect of the diffusion properties and geometries of polymeric seals on the gas leak behavior.

II. MOTIVATION: HELIUM FINE LEAK TEST RESULTS OF METAL-SEALED AND POLYMER-SEALED PACKAGES

The helium fine leak test has been practiced widely for hermeticity evaluation [8]–[17]. The conceptual idea of the helium fine leak test is to “bomb” the specimen with helium, i.e., subject it to pressurized helium for a period of time and then transfer it to a helium mass spectrometer to measure the rate at which the helium inside the package leaks out.

Hermeticity can be quantified by performing a regression analysis of the helium leak test data using the gas conduction-based governing equation [14], [15]. This technique has been successfully implemented to determine the true leak rates of metal-sealed MEMS packages, where the following closed-form equation was used for the regression analysis [14], [15]:

\[ R(t) = \Omega \exp \left( -\frac{l_a t}{V p_0} \sqrt{\frac{M_{\text{air}}}{M_{\text{He}}}} \right) \]  \hspace{1cm} (1)

where \( R \) is the apparent leak rate, \( \Omega \) is the initial apparent leak rate obtained at the helium spectrometer test, \( l_a \) is the true leak rate for air, \( V \) is the volume of the cavity, \( p_0 \) is a constant (1 atm), and \( M_{\text{air}} \) and \( M_{\text{He}} \) are the molar mass of air and...
helium, respectively. The true leak rate is a normalized gas flow rate under the pressure differential of unity (1 atm) between the package cavity and the ambient, while the apparent leak rate is the actual gas flow rate captured by the helium spectrometer.

Fig. 1 shows helium fine leak test results obtained from two separate tests with a metal-sealed package \( (V_{\text{cavity}} = 2.16 \times 10^{-4} \text{ cc}) \) and a polymer-sealed package \( (V_{\text{cavity}} = 3.1 \times 10^{-4} \text{ cc}) \). The test conditions include a bombing time of 6 h at 4 atm and a dwell time of 10 min. The results from the regression analysis using the gas conduction equations \([[1]]\) are also shown in Fig. 1. Nearly perfect correlation exists for the metal-sealed package while for the polymer-sealed package correlation starts to fail approximately after 1000 s. It should be noted that the regression was conducted in the linear scale for both data sets, and the result was plotted in the log scale to highlight the discrepancy of the polymer-sealed package at the later stage of testing.

Another set of helium fine leak tests was conducted to further elucidate the different physical behavior of the two packages. In the experiment, individual packages as well as batches containing multiple identical packages were tested; in the batch tests, 54 metal-sealed and 20 polymer-sealed packages were used. The signals obtained from the batch tests and single package tests are shown in Fig. 2(a) and (b) for polymer sealed and metal sealed packages, respectively. The batch test signals normalized by the number of packages in the batches are also plotted for comparison.

The normalized signal of the polymer-sealed packages is similar to that of the single package signal [Fig. 2(a)]. Additional tests of packages used in the batch test revealed that the polymer-sealed packages produced virtually the same signal when tested individually. On the other hand, the normalized signal of the metal-sealed packages is much lower than that of the single package signal [Fig. 2(b)], which indicates that the average signal of the batch does not represent the leak behavior of a single package. Additional tests confirmed that only five out of the 54 packages used in the batch test were leaky, and these packages produce unique apparent leak rate profiles [[14], [15]].

The aforementioned results clearly indicate the different gas transport mechanisms in the two packages. In metallic seals, gas transport occurs through a few nanoscale leak channels (gas conduction), and thus the leak rate depends on the gas molar mass and the geometry of the channel (diameter and length). Even when multiple nanoscale leak paths exist, they can be modeled as an effective single leak channel, and thus a regression analysis based on gas conduction equations can be employed to characterize the leak rate [[14], [15]]. On the other hand, gas transport in polymeric seals occurs through the bulk material (gas diffusion), and thus the leak rate depends on the gas diffusion properties (diffusivity and solubility) and the structure of polymer seals.

In fact, the diffusion analysis, which will be presented in detail later, showed that helium detected by the mass spectrometer was attributed mainly to the amount of helium diffused into polymer seals during bombing, whereas it was leaked out from the cavity through nanoscale channels in the case of metal-sealed packages. It is also important to note that leak rates of metal-sealed packages can be calculated for any other gas species at any temperatures from the helium leak test results (leak rates are inversely proportional to the square root of molecular weight but directly proportional to the square root of temperature [[12]]), but the helium leak data is absolutely no use for polymer-sealed packages simply because no simple relationship of diffusion mechanism among different gas species exists.
The gas transport in polymeric seals can be described only by the gas diffusion mechanism, which is the motivation of this paper.

III. GOVERNING EQUATIONS AND IMPLEMENTATION

A. Gas Diffusion Equations

In both molecular gas conduction and gas diffusion, the gas flux can be described by the gas conductance equation in its general form as [8]

\[ J = F \Delta p \]  

(2)

where \( J \) is the gas mass flux (in kilograms per square meter second), \( F \) is the gas conductance (in seconds per meter), and \( \Delta p \) is the gas pressure differential (in pascal). In the case of gas conduction, the gas conductance is derived from the kinetic theory of gases while it is determined from Fick’s first law in gas conduction, the gas conductance is derived from the kinetic theory of gases while it is determined from Fick’s first law in gas conduction. These expressions are [8]

\[ F = \frac{d_{tube}}{3L} \sqrt{\frac{8}{\pi M R_0 T}} \]  

(3)

for gas conduction

\[ F = \frac{P}{L} \]  

(4)

for gas diffusion

where \( d_{tube} \) is the diameter of a nanoscale leak channel (in meters), \( L \) is the conduction or diffusion path length (in meters), \( M \) is the gas molar mass (in kilograms per mole), \( R_0 \) is the universal gas constant (8.3145 J/mol · K), \( T \) is the temperature (in kelvin), and \( P \) is the permeability of the gas (in seconds). Although the two mechanisms are described by the same form of equations, there are two fundamental differences between them with regard to the geometry of gas transport paths and the time required for pressure gradient development inside the transport paths.

In gas conduction, gas molecules travel through a nanoscale channel and thus can be regarded as a Cartesian 1-D flow problem. The pressure gradient inside the flow channel is developed almost instantaneously, and transient effects are negligible. Thus, the gas transport can be predicted by simply considering the conduction equation \((2)\) with appropriate boundary conditions at both ends of the channel.

In contrast to gas conduction, gas diffusion takes place through the entire sealing area. Multidimensional modeling is necessary to account for the actual sealing layer structure. In addition, the gas pressure gradient inside the sealing material develops very slowly (usually on the order of hours to days). The conductance equation based on Fick’s first law cannot model such a slow pressure gradient development and hence Fick’s second law has to be considered.

Fick’s second law is derived from the principle of mass continuity for an infinitesimal volume as

\[ \frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) \]  

(5)

where \( C \) is the gas concentration (in kilograms per cubic meter), \( \nabla \) is the gradient operator, and \( D \) is the gas diffusivity. In gas diffusion, the gas transport can be described by the gas conductance equation in its general form as [8]

\[ (\partial p) / (\partial t) = D (\partial^2 p / (\partial r^2) + 1 / r \partial p / \partial r) \]  

(8)

The permeability \( P \) is defined as the product of solubility and diffusivity \((P = DS)\). As shown in (2) and (4), the permeability characterizes the steady-state gas flux through a polymer, thus can be measured from a gas transmission test. On the other hand, the diffusivity governs the transient gas transport inside the polymer, thus can be determined from a transient gas absorption/desorption/transmission test [8].

The cavity of a typical MEMS package has a rectangular (or square) shape. Many parameters are required to define the structure of the cavity and the surrounding seal, and hence the rectangular shape is not most ideal for a parametric study. In this paper, we consider an axisymmetric model, which is much more effective for the parametric study. Although simplified, the axisymmetric model effectively represents the gas diffusion behavior of the actual cavity structure.

B. Axisymmetric Formulation

An axisymmetric model is formulated to illustrate the transient boundary conditions. Its normalized form will be utilized later for an extensive parametric study. A schematic diagram of the axisymmetric model is shown in Fig. 3. The axisymmetric form of \((7)\) can be expressed as

\[ \frac{\partial p}{\partial t} = D \left( \frac{\partial^2 p}{\partial r^2} + \frac{1}{r} \frac{\partial p}{\partial r} \right) \]  

(8)

and the boundary and initial conditions are

\[ p(r_0, t) = p_a \quad p(r, t) = p_c \quad p(r, 0) = 0 \]  

(9)
C. Effective Volume Scheme

As shown in Fig. 4, a real 3-D package [Fig. 4(a)] can be modeled as a 2-D structure [Fig. 4(b)] since a cavity and a seal are sandwiched by an inorganic substrate or a silicon chip through which gas cannot penetrate or, if any, the amount is negligible. The 2-D diffusion model can be solved numerically using commercially available finite element analysis (FEA) software packages. It is important to recall that the boundary condition at the polymer seal and cavity interface [(9)] is transient; the cavity pressure increment at each time step should be calculated and subsequently used to update the boundary condition at the inner surface after each time step. This updating procedure requires a user-defined algorithm [18].

An effective modeling scheme is proposed to avoid the user-defined algorithm (this scheme will be referred to as “effective volume”). A schematic illustration of the effective volume scheme is shown in Fig. 4(c). It models the package cavity as an imaginary polymer with an extremely large diffusivity and an “equivalent solubility”. The large diffusivity (several orders higher than that of the polymeric seals) ensures that the gas pressure is uniform within the cavity. It is important to note, however, that the solubility of the imaginary polymer cannot be chosen arbitrarily. Instead, the effective solubility should be derived from the gas law and Henry’s law as

$$S_c = \frac{C}{p} = \frac{nR_0T}{V} = \frac{M}{R_0T}$$

where \( \rho \) is the gas density, which has the same dimension as the gas concentration (in kilograms per cubic meter; note that gas density can be interpreted as gas concentration inside the imaginary polymer), \( V \) is the gas volume (in cubic meter), and \( n \) is the number of moles (in mole).

The effective volume scheme transforms the original single material diffusion problem with transient boundary conditions into a bimaterial gas diffusion problem with fixed boundary conditions. Consequently, the Nernst distribution law should be considered in addition to mass continuity at the cavity–polymer seal interface [the inner surface of the polymer seal, \( x = L \) in Fig. 4(c)], which can be expressed as [19]

$$p(L) = \frac{C_c(L-)}{S_c} = \frac{C_p(L+)}{S_p}$$

where \( C_c \) and \( C_p \) are the gas concentration (density) of the cavity and the polymeric seal, respectively, and \( L- \) and \( L+ \) are the (identical) \( x \)-coordinate at the interface approached from the cavity side and from the seal side, respectively.

The effective volume modeling scheme can be readily implemented using commercial FEA software packages. Not all commercial FEA software packages offer the mass diffusion analysis function, but the current problem—namely, a diffusion analysis of a multimaterial system subjected to an isothermal condition—can be solved by the thermal diffusion (or heat transfer) analysis function adopting the well-established thermal-moisture diffusion analogy [20], [21]. With both analysis functions, the mass continuity [including the Nernst distribution law defined in (12)] is automatically satisfied at the interface, and the user-defined algorithm is not required. The accuracy of the proposed effective-volume scheme has been confirmed by a direct numerical solution of (8) using the finite difference method [18].

IV. EXPERIMENTAL VALIDATION BY OPTICAL LEAK TEST

The Fickian gas diffusion model proposed in this paper is verified by an optical leak test method. The basic principle of the optical leak test [13], [22], [23] is shown in Fig. 5. A MEMS package is first subjected to a pressurized gas (i.e., constant external pressure). As the gas leaks into the package, the pressure differential (i.e., the difference between the external pressure and the cavity internal pressure) changes over a period of time. This change in pressure differential induces a change in specimen deformation that is recorded experimentally as a function of time. The experimental data are converted to the pressure differential using the predetermined relationship between the pressure differential and the specimen deformation (calibration...
Fig. 5. Schematic illustration of the optical leak test.

Then, the time-dependent internal cavity pressure can be determined by subtracting the pressure differential from the known external pressure.

A. Experimental Setup

The optical/mechanical configuration is shown schematically in Fig. 6. The specimen is held inside a cylindrical stainless steel pressure chamber, which is provided with a window for direct viewing. The pressure vessel is mounted on a heavy-duty stage in order to prevent vibrations on account of forces exerted by the pressure tubing that supplies gas into the vessel. This stage offers $x$–$y$ translation and rotational adjustment of the vessel, and hence the specimen inside it as desired. The gas pressure is regulated by a PID controller (TESCOM ER3000).

The surface topography of the package is documented by a classical laser interferometry configuration called Twyman/Green interferometry [24]. The technique is simple and is ideally suited for MEMS packages since the package surface is specular, which is a critical requirement for the method. As shown in Fig. 6, two wavefronts from the specimen and the reference mirror interfere to form an interferogram (or fringe pattern). The interferogram provides a contour map of the surface topography. The fringe pattern is captured by a high-resolution camera (Pulnix TM-1040) through an imaging lens. The basic contour interval of this arrangement is $\lambda/2$, where $\lambda$ is the wavelength of the laser. For a helium neon laser ($\lambda = 632.9$ nm), the contour interval is 316.5 nm/fringe order. The fringe patterns are processed further by the fast Fourier transform (FFT) method [25] to enhance the displacement resolution.

The configuration used in the experiment offered the displacement measurement resolution of ±15 nm and the pressure regulation accuracy of ±0.3 psi (±0.02 atm). The details of the experimental setup can be found in [18].

B. Experimental Results and Validation

The package used in the experiment is shown in Fig. 7. It consists of a glass cap bonded to a silicon substrate using a photodefinable adhesive polymer. The cavity was fabricated through a lithography process. All the processes were conducted in a controlled nitrogen environment (0.9 bar). The height of the silicon substrate, the glass cap, and the polymer seal are 120, 500, and 46 $\mu$m, respectively. The overall package dimensions are 4.6 mm × 4.5 mm. The cavity dimensions are 2.22 mm × 2.86 mm, which yields an internal cavity volume of $\sim 3 \times 10^{-4}$ cc.

1) Calibration Curve: In order to obtain the calibration curve, the pressure in the chamber was increased to 4 atm (gauge) in steps of 0.25 atm, and the surface deformation was recorded at each step. Representative fringe patterns—(a) original and (b) modulated by a carrier pattern—and the corresponding (c) phase map and (d) 3-D map processed by the FFT method are shown in Fig. 8. The maximum deflections were determined from these 3-D plots. They were subtracted...
from the initial deflection to calculate the deformation-induced deflection corresponding to each pressure value. The deformation-induced deflections were used to obtain a relationship between pressure differential $\Delta p$ and the maximum deflection $W_{\text{max}}$ of the specimen as

$$W_{\text{max}} = 309.58(\Delta p) \quad (13)$$

where the units for pressure and deformation are in atmosphere and in nanometer, respectively. It is worth noting that the above relationship is valid for both bombing and release stages since the deformation is within the elastic range. This was confirmed again in the actual measurement for cavity pressure evolution.

2) Cavity Pressure Evolution: After the calibration curve was obtained, the package was subjected to a constant bombing pressure of 4 atm (gauge), and the deflections were measured as a function of time. The bombing pressure was maintained for 600 h. There was no noticeable deflection change after 600 h, indicating that the cavity pressure was equal to the bombing pressure. At this point, the “release” stage was initiated by closing the helium gas valve and opening the chamber to the atmospheric environment (0 atm of helium). The surface deflection was also documented regularly during the release stage. Representative fringe images and corresponding 3-D maps are shown in Fig. 9(a) and (b) for the bombing and release stages, respectively.

The effective deflections obtained from the 3-D maps are shown in Fig. 10, where the data points marked by a dotted circle were obtained from the results shown in Fig. 9. Using the calibration curve [(13)], the deflection values during the bombing and release stages were converted into pressure differential values. The internal cavity pressure was then calculated by subtracting these values from the known external pressure (4 atm while bombing and 0 atm during release) and is shown in Fig. 11.

3) Validation of Diffusion Mechanism: A finite element model based on the effective-volume scheme was built to simulate the cavity pressure evolution during the bombing and release stage. The modeling prediction is compared with the experimental data in Fig. 11. It is evident that the diffusion model follows the experimentally observed cavity pressure change extremely accurately. This corroborates the validity of the diffusion-based hermetic behavior of polymer-sealed MEMS packages and also validates the assumptions used in the boundary conditions for the finite element model.

It is to be noted that the two diffusion properties (diffusivity and solubility) required for the modeling were not known in advance. Instead they were varied systematically until the prediction shown in Fig. 11 was obtained. This process was
basically an inverse approach to obtain the unknown material constants. The details of the approach to determine the diffusion constants can be also found in [18].

V. FUNDAMENTALS OF GAS LEAK BEHAVIOR

A. Diffusion Regimes: Extreme Cases and Their Physical Implications

For a cavity enclosed by a polymeric seal, the diffusion equation can provide an approximate mass continuity relationship over the entire axisymmetric sealing structure as [26]

$$D_p S_p \frac{p_a - p_c}{L_p} \delta t \approx \delta p (S_p V_p + S_c V_c)$$

(14)

where $A_p$ is the area of the polymer seal at the center ($= \pi (r_i + r_o)h$; $h$ is the seal thickness), $\delta t$ is the time duration, $\delta p$ is the pressure rise during $\delta t$, $L_p$ is the width of the sealing layer ($= r_o - r_i$), $V_c$ is the cavity volume ($= \pi r_i^2 h$), $V_p$ is the polymer seal volume ($= \pi (r_o^2 - r_i^2)h$), $D_p$ and $S_p$ are the diffusivity and solubility of the polymer seal, respectively, and $S_c$ is the effective solubility of the cavity. The left-hand side of (14) is the amount of gas transferred through the polymeric seal and the right-hand side is the amount of gas accumulated in both the polymer and cavity. Rearranging (14) yields

$$\frac{\delta p}{\delta t} \approx \frac{D_p S_p (p_a - p_c)(r_o + r_i)}{L_p [S_p (r_o^2 - r_i^2) + S_c r_i^2]}.$$  

(15)

When $S_p (r_o^2 - r_i^2) >> S_c r_i^2$ or $R_S \equiv S_p (r_o^2 - r_i^2)/S_c r_i^2 >> 1$, (15) can be simplified as

$$\frac{\delta p}{\delta t} \approx \frac{D_p (p_a - p_c)}{L_p}.$$  

(16)

In this regime, the gas leak into the cavity is proportional to the diffusivity of the sealing polymer (will be referred to as diffusivity-dominant regime) and is inversely proportional to the square of seal width.

On the other hand, when $S_p (r_o^2 - r_i^2) \ll S_c r_i^2$ or $R_S \equiv S_p (r_o^2 - r_i^2)/S_c r_i^2 \ll 1$, (15) is simplified as

$$\frac{\delta p}{\delta t} \approx \frac{P_p (p_a - p_c)}{L_p S_c} \cdot \frac{r_o + r_i}{r_i^2}.$$  

(17)

In this regime, the gas leak is proportional to the permeability of the sealing polymer (will be referred to as permeability-dominant regime). Unlike the gas leak in diffusivity-dominant regime, it is also affected by the cavity size and the seal width.

It would be instructive to explain the physical implications of each extreme regime. In the diffusion-dominant regime, the maximum amount of gas that the cavity can hold is much smaller than the maximum amount of gas that can be absorbed in the seal. Since the effect of the cavity becomes almost negligible, the gas transport behavior of the entire structure becomes very similar to the single-material gas diffusion [7] where only diffusion properties are important.

In the permeability-dominant regime, the amount of gas inside the cavity becomes much greater than the amount of gas absorbed in the seal. The seal can be regarded as virtually an “empty” space with its original structure and properties. This seal space instantaneously reaches a pseudosteady-state condition with a linear pressure gradient since it takes almost no time for the gas to fill up the seal and to build up the gradient. Like the gas conduction mechanism, the transient effect becomes negligible. Thus, (2) and (4) become valid for this regime indicating that the gas transport should be dominated by the permeability of the seal.

B. Practical Implications of Diffusion Regimes

For a more effective parametric calculation, (8)–(10) are converted into nondimensional forms by normalizing independent variables ($r$ and $p$) with the outer radius ($r_o$) and the ambient pressure ($p_a$) as

$$\frac{\partial \tilde{p}}{\partial \tilde{t}} + \frac{1}{\tilde{r}} \frac{\partial \tilde{p}}{\partial \tilde{r}} = 0.$$  

(18)

$$\tilde{p}(1, \tilde{t}) = 1 \quad p(\tilde{r} = \tilde{r}_i) = \tilde{p}_c \quad p(\tilde{r} = 0) = 0.$$  

(19)

$$\tilde{p}_c (\tilde{t} + \Delta \tilde{t}) = \tilde{p}_c (\tilde{t}) - \frac{2 \tilde{r}_o S_p}{\tilde{r}_i S_c} \int_{\tilde{r} = \tilde{r}_i} \tilde{J} d\tilde{t}.$$  

(20)

where

$$\tilde{p} = \frac{p - p_a}{p_a} \quad \tilde{r} = \frac{r}{r_o} \quad \tilde{t} = \frac{D_p t}{r_o^2} \quad \tilde{J} = \frac{J r_o}{D_p S_p p_a}.$$  

(21)

The normalized form of the Nernst distribution law can be written as

$$\tilde{p}(\tilde{r}_i) = \frac{S_p}{S_c} \tilde{C}_c(\tilde{r}_i) = \tilde{C}_p(\tilde{r}_i +),$$  

(22)

where $\tilde{C} = \frac{C}{S_p p_a}$.

The normalized axisymmetric model is utilized to investigate the fundamental behavior of gas leak in polymer-sealed packages. Fig. 12 shows a normalized cavity pressure evolution obtained with various solubility ratios ($S_p/S_c$) when the radius ratio is 0.5 ($r_i = L_p$). It is interesting to note that all curves with...
the solubility ratios above 100 are superimposed while all those with the solubility ratios below 0.01 shift along the log time axis. They represent the two extreme cases discussed above.

At the diffusivity-dominant regime (high solubility ratios), the gas leak is not affected by the solubility of the sealing polymer [(16)], resulting in the identical pressure rise, as shown in Fig. 12. At the permeability-dominant regime (low solubility ratios), a time required to reach a certain cavity pressure is inversely proportional to the permeability of the sealing polymer [(17)], which results in a shift along the log time axis. It should be noted that the diffusivity remains constant for all plots in Fig. 12, and thus the solubility change is the same as the permeability change.

This trend is shown in Fig. 13, where the normalized time to reach half the ambient pressure as a function of $R_S$ is plotted for various radius ratios. The results show two distinct regimes; regimes with a constant nondimensionalized time (diffusivity-dominant regime) and a constant gradient (permeation-dominant regime). In order to determine the regimes more accurately, the slopes of the curves in Fig. 13 are calculated by differentiating the normalized time in the log–log scale. The results are shown in Fig. 14.

The regimes can be defined approximately using the plot in Fig. 14—the permeability-dominant regime as $R_S \leq 0.01$, the diffusivity-dominant regime as $R_S \geq 500$, and the transition regime as in-between. The range of $R_S$ for each regime varies only slightly with the radius ratio ($r_i/r_o$). The magnitude of $R_S$ now can be used as the metric of diffusion regimes.

The above extreme cases have two important practical implications. If a package is in the diffusivity-dominant regime, the solubility (or permeability) does not have to be measured since the diffusivity itself is sufficient to describe the gas leak behavior. Similarly, for a package in the permeability regime, only the permeability is required to predict the gas ingress into the cavity.

The proper determination of the regime can also help make a decision about which sealing material to be used for a given package design. A sealing material with the lowest permeability will provide the best sealing performance if the gas leak falls into the permeability-dominant regime. Similarly, if the gas leak is in the diffusivity-dominant regime, a sealing material with the lowest diffusivity will offer the best hermetic performance.

Since the metric of diffusion regimes $R_S$ was derived originally from the axisymmetric model, it cannot be directly applicable to a typical MEMS package with a rectangular (or square) cavity shape. A concept of “effective” radius is proposed to link the two different shape parameters. The effective radii can be defined simply by using the equivalent area as

$$r_{i,e} = \sqrt{A_i/\pi} \quad \text{and} \quad r_{o,e} = \sqrt{A_o/\pi}$$

where $r_{i,e}$ and $A_i$ are the effective radius and the area of the rectangle of the cavity, and $r_{o,e}$ and $A_o$ are the effective radius and the area of the rectangle of the package.

A supplementary numerical analysis confirmed that the internal cavity pressure change of packages with a rectangular seal can be predicted accurately by an equivalent circular seal with the effective radii when the width of polymer seal is constant. Accordingly, the diffusion regimes can be determined accurately by the effective radii. When the width of the rectangular polymer seal is significantly different in the horizontal and vertical directions, however, the gas permeation may not be uniform; the permeation is likely to happen through a thinner seal area. For these cases, the accuracy of the effective radii should be confirmed again.

C. Lag Time

When a fresh package is exposed to a gas, a certain amount of time (will be referred to as “lag time”) is required for gas molecules to travel from an ambient to a cavity. Actual gas leakage into the cavity begins after this lag time. Since it happens inside the polymer, it depends only on the width and diffusivity of the polymer seal. More specifically, it is proportional to the square of the seal width and inversely proportional to the diffusivity, which can be readily seen from a dimensional analysis, i.e., $[D] = [L]^2/[t]$, hence $[t] = [L]^2/[D]$.

Theoretically, the lag time can be defined as the time for the fastest gas molecule to travel through the shortest diffusion path.
in a polymeric sealing, which is extremely difficult to measure. In a practical point of view, the lag time can be defined as the time to accumulate a threshold value of gas amount that has an impact on the device performance or reliability.

Considering a normalized threshold value of 0.001 ($\tilde{p} = 0.001$), the normalized lag time $t$ as a function of $R_S$ is shown in Fig. 15 for the radius ratio of 0.5. If the diffusivity is $1 \times 10^{-7}$ mm$^2$/s and the package radius is 4 mm, the actual lag time ranges approximately from 300 to 40 000 h for $R_S = 10^3$ and $10^{-4}$.

In the traditional helium fine leak test, the package is bombed for a few hours before being transferred to the spectrometer. Due to the lag time which is usually much longer than the bombing time, the helium may not even enter the cavity of polymer-sealed packages during the bombing period. In fact, the test may only measure helium that has been absorbed in the polymer seal. As mentioned earlier, the analysis of such data can lead to erroneous inferences about the hermeticity of the package and the helium-based fine leak test should not be used for polymer-sealed packages.

D. Illustration of Water-Vapor Diffusion

Water vapor is known to be one of the most detrimental gases to MEMS device reliability. Its leakage characteristic is investigated by the proposed modeling scheme. It is reasonable to assume that water vapor obeys the gas law within the range of temperature considered in the implementation (below 100 °C). With this assumption, the effective water solubility of a cavity required for the numerical calculation can be calculated as $2.165/T$ (in kelvin) $\times 10^{-9}$ s$^2$/mm$^2$ from (11).

A diffusion analysis proceeded with actual temperature-dependent diffusion properties, which are known to follow the Arrhenius relationship as [19]

$$
D = D_0 \exp \left( -\frac{E_D}{R_0 T} \right)
$$

$$
S = S_0 \exp \left( -\frac{E_S}{R_0 T} \right)
$$

$$
P = DS = P_0 \exp \left( -\frac{E_p}{R_0 T} \right)
$$

(24)

\begin{table}
\centering
\caption{Arrhenius Coefficients for Diffusion Properties of PI and LCE Estimated From the Plots in [26] and [27], Respectively}
\begin{tabular}{|c|c|c|}
\hline
 & PI & LCE \\
$D_0$ (mm$^2$/sec) & 3.16 & 3.8$\times 10^{-5}$ \\
$E_D$ (J/mol) & 41990 & 14200 \\
$S_0$ (sec$^2$/mm$^2$) & 5.15$\times 10^{-16}$ & 5.30$\times 10^{-15}$ \\
$E_S$ (J/mol) & -43240 & -40600 \\
$P_0$ (sec) & 1.63$\times 10^{-15}$ & 2.01$\times 10^{-21}$ \\
$E_p$ (J/mol) & -1250 & -26400 \\
\hline
\end{tabular}
\end{table}

where $D_0$, $S_0$, and $P_0$ are diffusivity, solubility, and permeability constants, respectively, and $E_D$, $E_S$, and $E_p$ are the corresponding activation energy. Arrhenius coefficient of diffusion properties for generic polyimide (PI) and liquid crystal epoxy (LCE) found in the literature [27], [28] are listed in Table I.

An axisymmetric structure was used for the analysis ($r_1 = L_p = 2$ mm, $r_o = 4$ mm). The package was subjected to three ambient temperatures: 25 °C, 85 °C, and 121 °C for PI [26] and LCE [27] ($r_o = 4$ mm, $r_i = 2$ mm). The numbers on curves indicate diffusivity values ($\times 10^7$ mm$^2$/s) used in the analyses.

The $R_S$ values of three cases ranges approximately from 28 600 (25 °C, LCE) to 150 (121 °C, PI). This large range of $R_S$ values was attributed to the wide range of solubility ratio (Fig. 17). The cavity pressure evolution curves in Fig. 16 are shifted along the log time axis as the diffusivity changes. All cases fall within or near the diffusivity-dominant regime, where the gas leak behavior is dependent only on diffusivity regardless of solubility or permeability.

The above illustration shows that the water-vapor leakage will increase at elevated temperatures, as intended by the accelerated test standards. Some liquid crystal polymers for hermetic sealing applications are known to have extremely low solubility (two orders lower than generic polymers for
VI. CONCLUSION

Gas diffusion-based mechanism was proposed to describe the hermeticity of polymer-sealed packages. An effective numerical scheme was developed to solve the governing equations. The scheme was verified experimentally and further utilized to characterize the gas leak behavior in polymer seals. The results showed two important fundamental characteristics of gas transport in polymer-sealed packages: gas diffusion regimes and lag time. Three distinctive gas diffusion regimes were identified in terms of package structure and sealing polymer properties, and their practical implications on material property measurement and package design were described. The lag time (time duration for gas molecules to travel from an ambient to a cavity) is another unique characteristic of the diffusion-based gas transport mechanism in polymer-sealed packages. The numerical results for typical advanced polymers showed that the lag time ranges from several hours to hundreds of days depending on the polymer seal property and structure. The model was also applied to illustrate the water-vapor leak behavior of packages using the advanced polymers used in microelectronics devices. The gas properties of high-performance polymers for MEMS applications are not available in the literature and an extensive experimental and numerical study is warranted to establish a proper accelerated test guideline for polymer sealing materials.

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