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Effects of Vapor Pressure and Super-Hydrophobic Nanocomposite Coating on Microelectronics Reliability

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ABSTRACT Modeling vapor pressure is crucial for studying the moisture reliability of microelectronics, as high vapor pressure can cause device failures in environments with high temperature and humidity. To minimize the impact of vapor pressure, a super-hydrophobic (SH) coating can be applied on the exterior surface of devices in order to prevent moisture penetration. The underlying mechanism of SH coating for enhancing device reliability, however, is still not fully understood. In this paper, we present several existing theories for predicting vapor pressure within microelectronic materials. In addition, we discuss the mechanism and effectiveness of SH coating in preventing water vapor from entering a device, based on experimental results. Two theoretical models, a micro-mechanics-based whole-field vapor pressure model and a convection-diffusion model, are described for predicting vapor pressure. Both methods have been successfully used to explain experimental results on uncoated samples. However, when a device was coated with an SH nanocomposite, weight gain was still observed, likely due to vapor penetration through the SH surface. This phenomenon may cast doubt on the effectiveness of SH coatings in microelectronic devices. Based on current theories and the available experimental results, we conclude that it is necessary to develop a new theory to understand how water vapor penetrates through SH coatings and impacts the materials underneath. Such a theory could greatly improve microelectronics reliability.

KEYWORDS vapor pressure, moisture, semiconductor reliability, microelectromechanical systems (MEMS), super-hydrophobic, nanocomposite coating

1 Introduction

As the components of microelectronic devices are produced globally in different regions, it is inevitable that microelectronics materials, such as polymeric encapsulants and die-attach thin films, would absorb a certain amount of moisture from humid ambient environments during transportation and storage. The moisture absorbed can be detrimental to device reliability, eventually causing deleterious effects such as material aging [1], hygroscopic swelling, interfacial weakening and delamination [2–4], and suppression of material strength [5–7]. Moreover, during the soldering reflow process, the entire packaged device must be exposed to very high temperatures of up to 220–270 °C. Therefore, the moisture absorbed by polymer materials in the device will experience a phase change and extremely high internal vapor pressure can be generated. As a result, the polymer material is stressed under the combined vapor pressure and thermal stress, resulting in popcorn-like failures [3].

To reduce moisture uptake and potential damage caused by high vapor pressure, surface coating can be applied to packaged devices, such as super-hydrophobic (SH) coating with nanocomposites technology [8–12]. The general rules for designing SH surfaces are: ① to minimize the surface energy and ② to increase the surface roughness. Surfaces coated with SH materials usually have excellent water-repelling properties and display a large water contact angle (> 150°) with small hysteresis (< 10°) [8, 9, 13]. Similar surfaces can be found on many natural objects, such as lotus leaves [14]. These surfaces generally combine micro and nano roughness with low free-energy coatings [15]. Although SH coating is potentially a low-cost and highly reliable microelectronic packaging solution, moisture absorption after coating was still reported [16]. The underlying mechanism of such moisture absorption, however, could not be explained by current theories of moisture transport.

In this paper, we describe the existing methods that enable the evaluation of vapor pressure within polymers, with

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the intention of connecting the vapor pressure of water to the effectiveness of SH coating. We also discuss the methods used to generate an SH surface, followed by a discussion of interesting absorption behaviors after SH coating under various ambient conditions.

2 Vapor pressure modeling

High vapor pressure is considered to be the dominant cause of device failures (see Figure 1 for die-attach thin-film ruptures). Modeling vapor pressure and vapor flow may also help researchers to fully understand moisture transport in materials that are coated with SH nanocomposites. Therefore, many theoretical models have been developed to address vapor pressure and the related reliability issues [17–20]. In the following discussion, we present two different approaches, both of which have been successfully used to explain experimental tests. Since vapor pressure is always associated with moisture behaviors, the relationship between vapor pressure and moisture concentration becomes the key characteristic of different vapor pressure models.
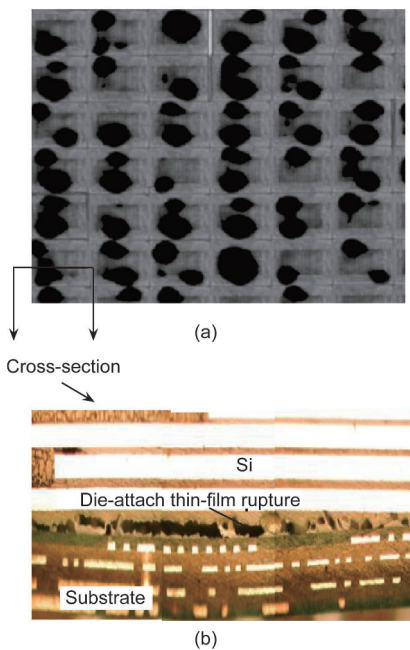

(a)

Cross-section

Si

Die-attach thin-film rupture

Substrate

(b)

Figure 1. (a) A scanning acoustic microscopy image on a 6 × 6 array chip scale package (CSP) panel (black regions mean failures inside packages); (b) die-attach film cracking and voiding at the bottom layer where it is attached to the substrate.

2.1 Micro-mechanics-based whole-field vapor pressure model

A whole-field vapor pressure model has been developed to predict vapor pressure during soldering reflow processes, and has been successfully applied to many problems [19]. Since most microelectronic materials are typically polymer composites, the model assumes that most of the absorbed moisture collects at the voids or polymer-filler interfaces [16]. Because it has been found that the moisture density in voids can be several orders higher than the ambient moisture density, it is concluded that a liquid form of water exists within the materials [19]. Consequently, there must be two distinct states of water existing in polymers: a purely vapor phase and a mixture of liquid and vapor phases, as shown in Figure 2.
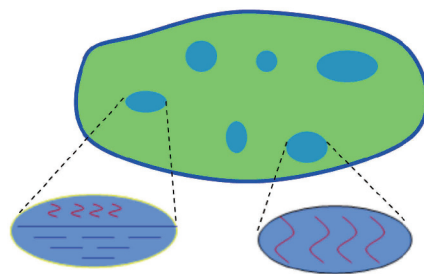

Figure 2. A schematic of a polymeric material with two different states of moisture in its pores [5].

By introducing porosity ϕ, the density (ρ) of the moisture absorbed in the materials can be calculated as

$$\rho = C/\phi \qquad (1)$$

where C is moisture concentration. Moisture concentration can be obtained by solving the transient moisture diffusion equation, which is based on Fick's law and is provided here:

$$\dot{C} = -\nabla \cdot (-D\nabla C) \qquad (2)$$

where D represents the moisture diffusivity. Porosity is usually an intrinsic material property that ranges from 1% to 10% for typical polymers.

The calculation of vapor pressure starts with determining the state of moisture in the voids. If the voids contain only vapor and the vapor pressure reaches the saturation point, the saturated moisture density, ρ_g, can be expressed according to the ideal gas law:

$$\rho_g(T) = \frac{p_g(T)}{RM(H_2O)T} \qquad (3)$$

where $\rho_g(T)$ is the saturated vapor pressure at a given temperature; the gas constant $R = 8.314 \ \text{J} \cdot (\text{mol} \cdot \text{K})^{-1}$, and the water molar mass $M(H_2O) = 18 \ \text{g} \cdot \text{mol}^{-1}$. The vapor pressure can then be evaluated by comparing ρ with ρ_g:

$$p(T) = \begin{cases} \dfrac{RT}{M(H_2O)\phi} \cdot C, \ \rho < \rho_g \\ p_g(T), \ \rho \geq \rho_g \end{cases} \qquad (4)$$

Note that the above equations are still valid if thermal expansion exists due to temperature change. For such a situation, the moisture concentration may change with the change of material volume, which can be calculated by the following relation:

$$dV/dV_0 \approx 1 + 3\alpha\Delta T \qquad (5)$$

where ΔT is the temperature difference and α is the coefficient of thermal expansion. Thus, the moisture concentration after expansion becomes:

$$C = dm/dV = \frac{dm}{dV_0}\frac{dV_0}{dV} = C_0(1 - 3\alpha\Delta T) \ (6)$$

where dm is the moisture mass and dV is the representative element volume.

The whole-field vapor pressure model includes a new field variable ϕ, which stands for the fraction of void volume. Clearly, accurate prediction of vapor pressure relies on void deformation, and the coupling of the vapor pressure model with solid deformation is needed. It is a well-accepted fact that the growth and coalescence of micro-voids in a packaging material will lead to mechanical failures of microelectronic devices (e.g., interface delamination and "popcorn" cracking).

Figure 3 gives examples of using the whole-field vapor pressure model. Based on the modeling results [6], two major factors can be identified: the reflow profile and the substrate thickness. It was found that the reflow profile can be carefully designed to meet the Joint Electron Device Engineering Council (JEDEC) standard and to lower the failure rate. As can be seen in Figure 3(a), under reflow profile a (which has a slow ramp rate), there is a transition point for moisture from binary state to a single vapor state, and the vapor pres-